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## **SIMMAX: A modern analog technique to deduce Atlantic sea surface temperatures from planktonic foraminifera in deep-sea sediments**

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**Abstract.** We present a data set of 738 planktonic foraminiferal species counts from sediment surface samples of the eastern North Atlantic and the South Atlantic between 87°N and 40°S, 35°E and 60°W including published Climate: Long-Range Investigation, Mapping, and Prediction (CLIMAP) data. These species counts are linked to *Levitus's* [1982] modern water temperature data for the four caloric seasons, four depth ranges (0, 30, 50, and 75 m), and the combined means of those depth ranges. The relation between planktonic foraminiferal assemblages and sea surface temperature (SST) data is estimated using the newly developed SIMMAX technique, which is an acronym for a modern analog technique (MAT) with a similarity index, based on (1) the scalar product of the normalized faunal percentages and (2) a weighting procedure of the modern analog's SSTs according to the inverse geographical distances of the most similar samples. Compared to the classical CLIMAP transfer technique and conventional MAT techniques, SIMMAX provides a more confident reconstruction of paleo-SSTs (correlation coefficient is 0.994 for the caloric winter and 0.993 for caloric summer). The standard deviation of the residuals is 0.90°C for caloric winter and 0.96°C for caloric summer at 0-m water depth. The SST estimates reach optimum stability (standard deviation of the residuals is 0.88°C) at the average 0- to 75-m water depth. Our extensive database provides SST estimates over a range of -1.4 to 27.2°C for caloric winter and 0.4 to 28.6°C for caloric summer, allowing SST estimates which are especially valuable for the high-latitude Atlantic during glacial times.

### **Introduction**

Progress in modelling past climatic changes [Gates, 1976; Imbrie and Imbrie, 1980; Kutzbach and Guetter, 1986; Berger and Labeyrie, 1987; Lautenschlager et al., 1987; Maier-Reimer and Hasselmann, 1987; Berger et al., 1989; Herterich, 1991; Heinze and Maier-Reimer, 1991; Maier-Reimer and Mikolajewicz, 1991] requires an equivalent advancement in the precision and reliability of paleoclimatic proxy data to test the models [cf. Ravelo et al., 1990]. One of the most important paleoclimate data sets used in climate models is sea surface temperature (SST). The transfer technique to derive SSTs, based on quantitative counts of microfaunal components, has been established worldwide [Climate: Long-Range Investigation, Mapping, and Prediction (CLIMAP), 1981, 1984; Guiot, 1991].

The CLIMAP transfer function method [Imbrie and Kipp, 1971] was highly successful in generating a SST database that revolutionised concepts of global climate change. In regional restricted areas, however, this technique suffers from so called "no-analog sample problem"; that is, past species assemblages which significantly deviated from the modern faunas cannot be fitted

into the modern SST regression model. This caused data gaps and reduced resolution in many deep-sea sediment SST records. Moreover, the selection of the faunal end-members, the "factors", as a base for the regression is either arbitrary or to some extent biased. Recent work [McIntyre et al., 1989; Molino, 1992; Prell, 1985] used the modern analog technique (MAT), which is fundamentally different from the CLIMAP method, based on the degree of dissimilarity between fossil and modern faunal assemblages in a specified SST range.

Both temperature estimation approaches are based on a series of assumptions, which are discussed in detail by Imbrie and Kipp [1971] and Prell [1985]. The main assumptions are the ecology of the species assemblages has not changed since the time of the predicted SST estimates; the faunal composition of the sediment surface is systematically related to the SST, the seasonal SSTs are linearly related to ecologically significant aspects of the surface water masses; caloric winter and summer are not principally different on both the northern and southern hemispheres of the Atlantic; and the caloric winter or cold season is defined to be always colder than the caloric summer. This makes some problems in the tropics, especially in regions with cold summer upwelling. For the SIMMAX approach (SIMMAX is an acronym for a modern analog technique using a similarity index), we assume further that the mutual distribution patterns of the main faunal provinces are rather conservative.

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Our objective within the European Project of Oceanic Climate and Hazards (EPOCH) was to develop a SST estimation technique based on the MAT and to compile a common data set of all available assemblages of modern planktonic foraminifera from sediments of the Atlantic Ocean.

The workers on modern planktonic foraminifera generally follow the previous works of Parker [1962] and Bé [1977]. There are, however, minor problems with the initial statistical bases of these estimates, as the core-top data set combines results from different research groups, each with their own taxonomical interpretations. To find a common database, we reduced the number of species to 26 (Table A1<sup>1</sup>) by combining coiling variants of *Globorotalia truncatulinoides*, lumping *Globorotalia menardii* and *Globorotalia tumida*, and adding the artificial "P-D-intergrades" [Kipp, 1976] to *Neogloboquadrina pachyderma* var. *dextra*. Taxonomical problems will be discussed below.

The composition of a faunal assemblage in marine sediments is the result of the interaction of many environmental and dissolution processes of which SST is one of the most significant and best known parameters primarily reflecting oceanic climate and surface circulation [Levitus, 1982]. To estimate SST, both a reliable sediment surface database and accurate, reliable, and detailed modern oceanographic data are required. Previous studies of the Atlantic [Kipp, 1976; Thiede, 1977; Pujol, 1980; Pflaumann, 1985] have been based on classical atlas values [U.S. Naval Oceanographic Office, 1967]; these can now be replaced by the (more objectively analyzed) worldwide data sets of Levitus [1982]. Our seabed faunal database has been significantly enlarged by numerous additional samples whose quality has been greatly enhanced using modern techniques to sample the actual sediment surface by spade box and multicorers. Precise age determination (accelerator mass spectrometry (AMS) <sup>14</sup>C datings) has also helped to pick samples which represent the actual modern sediment surface [Winn et al., 1991]. To produce a large core-top database (Figure 1) we have combined our data with that of SPECMAP archive 1 [1989/1990] (for "SPECMAP" contact Data Support Section, National Center for Atmospheric Research, Boulder, Col.), which has also been carefully checked for consistency [Kipp, 1976; Imbrie et al., 1989; McIntyre et al., 1989].

Our main aim is to define a statistically significant relation between the sea surface temperatures and the planktonic faunal composition on the seafloor, a relation that can be used for a prediction of past SSTs. The distributions of the living faunal assemblage in the uppermost water layers are strongly related to the sea surface water masses [Bé and Tolderlund, 1971], which themselves are mainly defined by their temperatures. The shell-producing period of the planktonic foraminifera is in the range of months [Hemleben et al., 1989]. After reproduction or death the empty tests rain down to the seafloor and are preserved in the sediment as record of the conditions of their habitat. This settling time is short compared to burial time into the sediment. The sediment faunal composition thus represents proxy data of many annual cycles, triggered by perennial, more or less constant ecolog-

<sup>1</sup>An electronic supplement of this material may be obtained on a diskette or Anonymous FTP from KOSMOS.AGU.ORG. (LOGIN to AGU's FTP account using ANONYMOUS as the username and GUEST as the password. Go to the right directory by typing CD APPEND. Type LS to see what files are available. Type GET and the name of the file to get it. Finally type EXIT to leave the system.) (Paper 95PA01743, SIMMAX: A modern analog technique to deduce Atlantic sea surface temperatures from planktonic foraminifera in deep-sea sediments, Uwe Pflaumann, Josette Duprat, Claude Pujol, and Laurent D. Labeyrie). Diskette may be ordered from American Geophysical Union, 2000 Florida Avenue, N.W., Washington, DC 20009; Payment must accompany order.

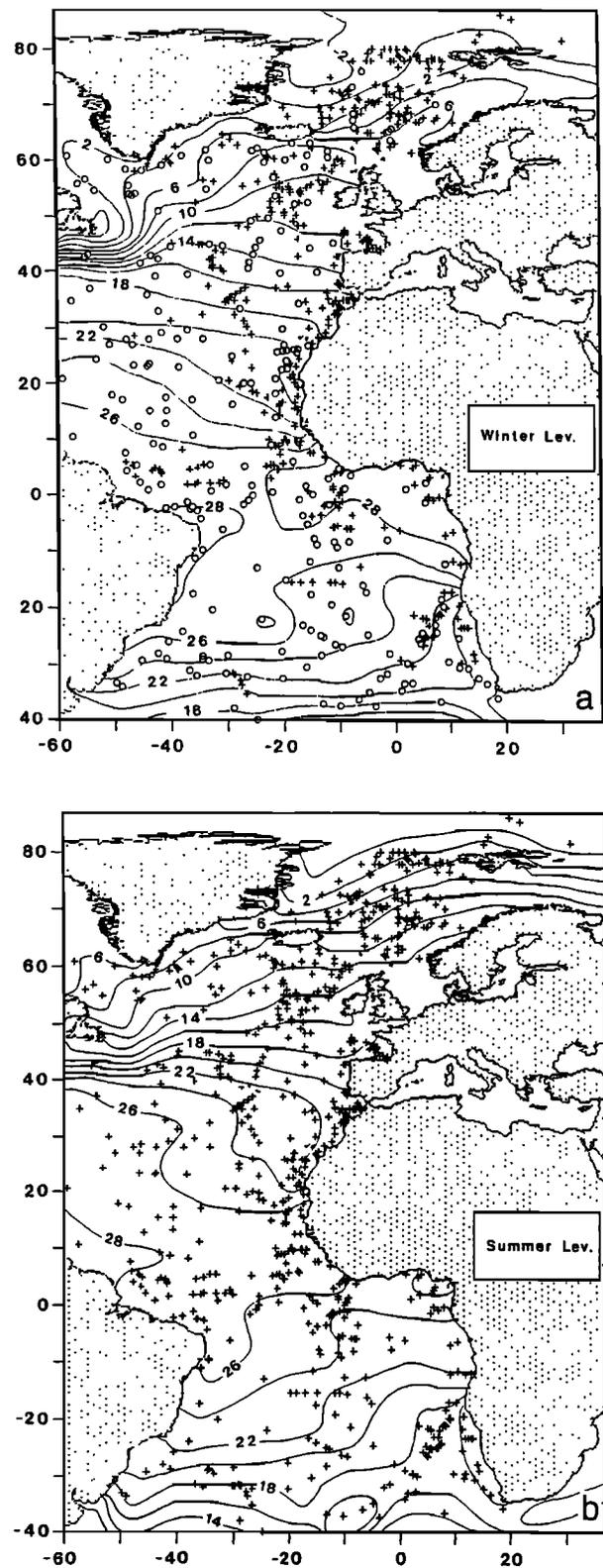


Figure 1. Location of 738 sediment surface samples used for the SIMMAX technique and sea surface temperature (SST) of Levitus [1982], derived from the original 1x1° grid: (a) northern hemisphere winter; (b) northern hemisphere summer. Circles mark SPECMAP data.

ical conditions. Depending on accumulation rate, preservation, and bioturbation, a 1-cm-thick section of otherwise undisturbed pelagic sample contains the integrated record of generally, at best, no less than 100 years.

Modern temperature observations of the sea surface have been made for about 100 years [Levitus, 1982], similar to the integrated duration of the core-top samples. This allows us to determine significant relationships between these (multiple) integrated annual records of faunal production and seasonal long-range integrated mean temperatures, although a statistically significant correlation between the two data sets does not prove the implied causal relationships [e.g., Cline and Hays, 1976; Overpeck et al., 1985].

Because previous regionally restricted SST transfer functions gave a high number of glacial no-analog faunal samples in tropical cores [Pflaumann, 1986; Brassell et al., 1986], we decided to use the "modern analog" technique (MAT) [Hutson, 1977a, b; Hutson and Prell, 1980; Prell, 1985] as a standard ocean-wide approach. In addition, we compare the MAT results with the results from the CLIMAP transfer function method [Imbrie and Kipp, 1971; Kipp, 1976] in order to ascertain the differences in the SST estimates of both methods.

The MAT procedure does not automatically exclude no-analog samples. However, it indicates them by low average similarity coefficients (as "similarity" is the positively expressed alternative of the negatively expressed dissimilarity, we prefer to use the term similarity). The low averages may be because the samples in question truly are "no-analog" (having no core-top equivalents) or because there are fewer than 10 (or whatever cut-off number is chosen) "good" analogs. Similarly, the CLIMAP transfer technique may indicate no-analog conditions by low communality values. This situation requires some thought on the

part of the analyst: there is no automated computational procedure for deciding how or if a given ancient sample can be used for a valid paleoenvironmental interpretation. With increasing numbers of poor analog samples, the similarity index tends to become zero [Overpeck et al., 1985]. So SST estimates based on faunal communities therefore need to be treated with special care (1) if the similarity index is low, (2) if the standard deviation of the selected mean values of the scalar products is high, or (3) if a parallel evaluation by the CLIMAP transfer technique method signals a no-analog situation. Otherwise, if just two independent transfer methods like SIMMAX and CLIMAP transfer technique are applied to the same data set and result in a similar set of proxy data, our belief in the credibility and the reliability of the relationship between the faunal composition of planktonic foraminifera and the SST will strongly increase.

To critically evaluate the data, we started to investigate samples collected by the Kiel and Bordeaux/Gif working groups in terms of consistence of the areal distribution of the various faunal components and modern SST values. This calibration data set has been progressively enlarged. Samples that significantly increased the variance of the data set have been carefully checked for the validity of their attributed modern-age assignment by searching for other AMS-<sup>14</sup>C dated cores in their vicinity. Application of two different methods of SST estimation technique (MAT versus factor and regression analysis) increased the precision and reliability of our results, because internal discrepancies in the data set could be detected and thus eliminated.

The previous attempts to estimate Atlantic SST from foraminiferal faunas can be judged on their summary statistics (Table 1) indicating the various approaches to refine the results during the last decades.

**Table 1.** Summary Statistics of Selected Techniques to Estimate Sea Surface Temperature (SST) by Planktonic Foraminifera in the Atlantic

Reference	<i>Imbrie and Kipp</i>	<i>Kipp</i>	<i>Thiede</i>	<i>Pflaumann</i>	<i>Prell</i>	<i>Mix et al.</i>	<i>Ruddiman and Esmay</i>	<i>Dowsett and Poore</i>	This Paper
	[1971]	[1976]	[1977]	[1985]	[1985]	[1986]	[1987]	[1990]	
Acronym	-	F13	-	134/6	ANALOG8 8 squared chord distance	FA20	F13x5	GSF18	SIMMAX
Region	North Atlantic	North Atlantic	eastern North Atlantic	eastern low latitude Atlantic	Atlantic part of World Ocean	tropical Atlantic	subpolar North Atlantic	North Atlantic	eastern North and South Atlantic
Age since	Pleistocene	Pleistocene	Pleistocene	Pleistocene	Pleistocene	Pleistocene	Pleistocene	Pliocene	Pleistocene
Taxonomic categories	22	29	19	19	31	29	5	18	26
Factors/NNN	5	6	5	6	10 NN	6	5	5	10 NN
Calibration points	61	191	89	134	356	357	129	223	738
SST caloric winter									
Correlation coefficient	0,986	0,991	not given	0,98	0,99		0,967	0,96	0,99
Std. error		1,165	not given	1,18	1,02	1.2 (annual)	1,82	1,47	0,9
minimum SST estimate	-0,1	0	7,9	8,1	0,7	does not fit	0,5	0	-1,4
maximum SST estimate	26,2	26	25,5	27	25,3	does not fit	does not fit	26	27,2
SST caloric summer									
Correlation coefficient	0,964	0,985	not given	0,97	0,99	does not fit	0,957	0,96	0,99
Std. error		1,38	not given	1,2	0,98	does not fit	2,25	1,36	0,96
minimum SST estimate	5,9	5,9	11,5	11,5	5,3	does not fit	6	2	0,4
maximum SST estimate	28	28	27,1	28	27,7	does not fit	does not fit	27	28,6

NN is the number of best analogs; std. error is the square root of the variance of the residuals.

## Methods

### Faunal Analysis

We followed the convention of the CLIMAP group in analyzing the >150- $\mu\text{m}$  sediment size fraction and whenever possible counted a split of at least 300 specimens per sample. Only in exceptional cases of poor regional sampling density was the minimum set to >250 specimens to allow those samples into the data set.

For samples containing extremely dominant left-coiling *Neogloboquadrina pachyderma* the standard counting procedure was changed in order to exclude statistical white noise due to insufficient counts for the nonpachyderma faunal components. Here the counting limits were raised up to 2500 specimens per sample. The minimum number was calculated as

$$n = N/(1+a*a*N)$$

[Sachs, 1984, p. 265, formula 4.31] where  $n$  is the minimum number,  $N = 10,000$ ,  $a$  is deviation, and  $a*a$  refers to a tolerance limit significant at the 5 % level.

In four cases (stations 21298-3, 21299-1, 21530-3, 23232-1), the minimum number was not reached. In order to retain the information from these extremely polar samples, the value of left-coiling *N. pachyderma* was set to 100%.

Additional faunal counts from the Greenland-Norwegian Sea indicate only a minority of samples containing 100 % left-coiling *N. pachyderma* (Figure 2). Beyond the limit of permanent ice coverage, the planktonic foraminiferal faunal content in modern seafloor samples is too small to be used for SST estimates. It can be shown that the Arctic front is documented by the transition between 90 and 94% left-coiling *N. pachyderma*, while values of about 98 % follow the polar front.

Finally, our surface data set contains 738 samples of which 29 sample counts are based on at least 250 specimens, while the other 709 sample counts are based on at least 300 specimens (data available from Past Global Changes (PAGES) marine data repository SEPAN; see Acknowledgments section for information on how to access this data). To make the counting and determination procedure easier, the >150- $\mu\text{m}$  size fraction of a part of the samples was subdivided into 150-200, 200-250, 250-315, 315-500, and >500- $\mu\text{m}$  size fractions. These subsamples were then each further subdivided into suitable portions for counting by an OTTO microsampler. The counts of all subfractions (containing generally more than 100 specimens) are then combined to obtain the overall species percentages of the respective sample. By this procedure the grain sizes studied under the binocular microscope at anyone time are more similar, enabling a quicker and more reliable species determination of all specimens. The error which is introduced by this procedure is comparable with, or lower than that of first splitting down the whole fraction >150  $\mu\text{m}$  and then sieving [cf. Sarnthein, 1971].

In order to estimate the actual personal or procedured bias in the counting procedure, 16 samples were counted using two different methods; first by splitting and then sieving, and second by sieving and then splitting. The linear correlation coefficient between both estimates of SST is 0.92 for caloric summer and 0.91 for caloric winter (Figures 3a and 3b), the mean of the deviations are  $-0.2^\circ\text{C}$  for winter and  $-0.01^\circ\text{C}$  for summer, and the standard deviations of the residuals are  $2.1^\circ\text{C}$ . Because of the unrepresentative low number of test samples it is not allowed to transfer this "error of the error" to the whole data set. Thus both procedures generate results which are within the error range of the standard deviation.

To compare the differences of the two counting procedures, one sample (1510) was treated by both procedures:

First, the sample was sieved into seven size fractions; then each size fraction was split into halves  $x$ -times so that the sum of planktonic foraminifera counted in all subfractions was about 300 specimens.

After counting, the number of specimens thus has to be multiplied by  $2^x$  to obtain the original number per species and fraction of the entire sample volume. These counts per fraction were summed up to calculate the sum of planktonic foraminifera per sample. Finally, these species counts were divided by the total number of planktonic foraminifera to obtain the species percentages.

For each of the six size fractions the above procedure was repeated seven times, replacing the splits into the original fraction after counting, thus resulting in  $7^6 = 117,649$  possible combinations of the SIMMAX caloric winter and summer temperatures to be calculated. The minimum and maximum temperatures differ by  $0.4^\circ\text{C}$  for caloric winter SST and by  $0.3^\circ\text{C}$  for caloric summer SST.

Second, the sample was split seven times; the subsample was sieved into six grain size classes and counted. By the sum of the counts of each species the percentages of the fauna were calculated. The whole procedure was repeated eight times.

According to the statistics of the second approach the maximum winter SST differences are  $0.4^\circ\text{C}$  and the maximum summer SST differences are  $0.1^\circ\text{C}$ . (All raw counting data are available on request from the German PAGES marine data repository SEPAN (see Acknowledgments section)).

The minimum number of faunal taxa used partly depended on the taxonomy of previously published foraminiferal data used in this study [Pflaumann, 1975; Kipp, 1976; Thiede, 1977; Pujol, 1980; Duprat, 1983; Pflaumann, 1985] and partly on the taxonomy of older core counts (Table A1). To reduce the statistical noise by rare species, we limited the number of taxa to 26 categories.

Our taxonomy closely follows that of Bé [1977]. The most pertinent taxonomic problem is the definition and thus the identification of the intergrades between right-coiling *Neogloboquadrina dutertrei* and *N. pachyderma* var. *dextra* (*N. dutertrei* indicates a tropical environment, while *N. pachyderma* var. *dextra* indicates a subpolar environment). Our taxonomic strategy was to reduce the number of intergrades as much as possible and to include them with *N. pachyderma* var. *dextra* during the counting process. The intergrades identified in the SPECMAP data were added to the *N. pachyderma* var. *dextra*, though Kipp [1976] included some juvenile *N. dutertrei* in her "p-d" intergrade category. This may result in an artificial bias toward a warmer mean temperature range of *N. pachyderma* var. *dextra* (Figures 4a - 4d).

Another problem is the discrimination between *Globorotalia menardii* and *Globorotalia tumida* in fossil samples. To overcome this problem, we have combined these species to a single common taxon like Dowsett and Poore [1990]. The modern temperature range of both single taxa and their combination (Figures 5a - 5d) shows only minor differences within their temperature ranges.

### Age Control, Recognition of True Surface Samples, and Influence of Dissolution

Surface samples which have been directly AMS- $^{14}\text{C}$  dated or dated by AMS- $^{14}\text{C}$  analogs [Winn et al., 1991; M. Sarnthein, personal communication, 1993] and found not to be Recent were removed from the input matrix. Since in high-temperature tropical regions, menardiform species are common to abundant in sediment surface samples [Ericson and Wollin, 1968; Thiede, 1971], samples in the tropics with missing menardiform species

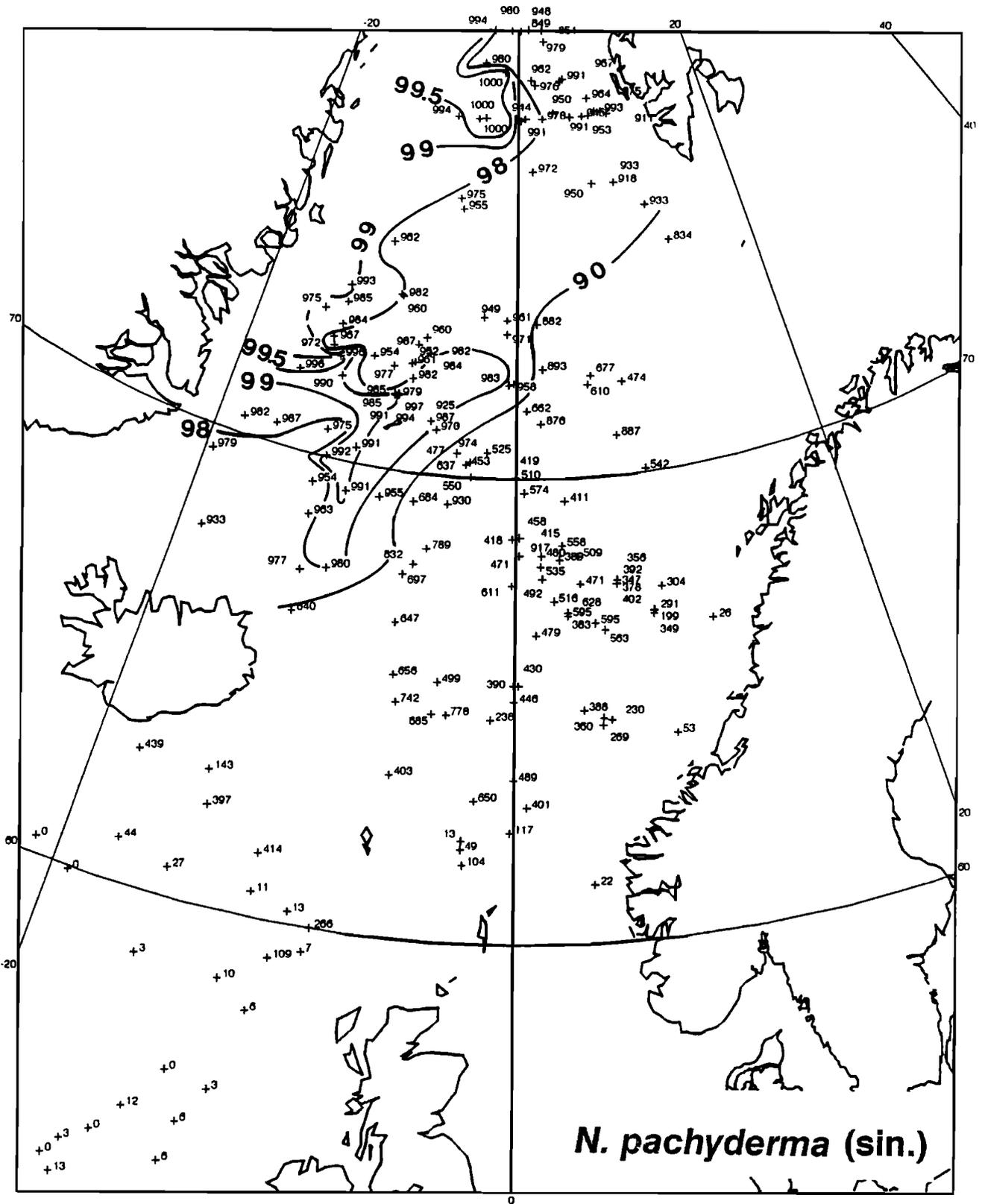
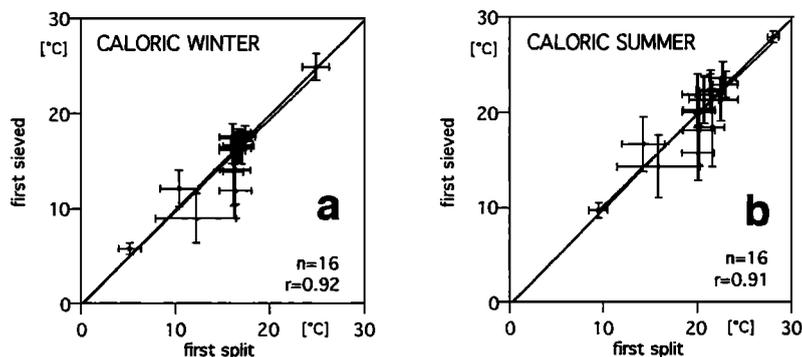


Figure 2. Areal distribution of the percentages of left-coiling *N. pachyderma* in total planktonic foraminifera of the pelagic sediments in the Norwegian-Greenland Sea. Isolines fitted by eye. (Small numbers at the stations in percent x 0.1).



**Figure 3.** Comparison of the SST estimates based on 16 samples counted twice. The x-axis shows estimates of samples which had been split first, then sieved; the y-axis shows estimates from samples which had been sieved first and then split: (a) caloric winter; (b) caloric summer. The error bars indicate the standard deviation of the 10 most similar analogs.

are considered as fossil and excluded from the input matrix. Samples from the transitional area containing left-coiling *Globorotalia hirsuta* were also considered as fossil [Pujol and Caralp, 1974; Pujol, 1975; Duprat, 1983] and excluded from the input matrix.

Before generating transfer functions, an initial simple scatter plot between temperatures and the faunal percentages indicates the temperature range and preference of the faunal components; moreover, it helps to identify misinterpreted faunas and/or simple data input errors. The temperature ranges and preferences of the important species also help to quantify the relation between SST and faunal components in the seafloor sediments [Loubère, 1981, 1982] and have allowed us to greatly improve the original evaluations for the Atlantic Ocean by Bé and Tolderlund [1971]. Labeling the data points by their station names means outliers can easily be detected either due to errors in the age determination or the temperature assignment. Analysis of the data set reveals two major types of outliers.

1. The first type is samples from the continental shelves, showing unusual faunal compositions, in most cases caused by redeposition and/or winnowing. Redeposition and winnowing do alter faunal compositions by adding or subtracting components to or from the respective fauna. Referring to count of planktonic foraminifera, it is not always possible to differ between allochthonous and autochthonous components. But, in case of inconsistency with the total data set, a reexamination of the sample also on components other than planktonic foraminifera will help for an explanation.

2. Samples from water depths below the lysocline which are affected by selective dissolution [Ruddiman and Heezen, 1967; Berger, 1970; Thunell and Honjo, 1989] enrich the faunal composition by dissolution resistant species. Extreme outliers within these samples were not included into the final modern analog data set (archived at the PAGES marine data repository SEPAN; see Acknowledgments chapter). Nevertheless, the final modern analog data set contains samples of nearly all classes of dissolution (Figures A1a and A1b), and deviations of the SIMMAX estimated SSTs from the measured *Levitus* [1982] derived SSTs cannot be explained by the influence of the selective dissolution only.

### Temperature Database

The "measured" sea surface temperatures were extracted from *Levitus* [1982]. (Note that the oceanographic seasons differ from the meteorological ones, the oceanographic northern winter sea-

son covering February, March, and April). To cover both hemispheres, we used caloric seasons, the cold season always being colder than the warm season [Kipp, 1976; Prell, 1985]. A full set of temperatures for four seasons at four depth ranges (0, 30, 50, 75 m) and their combined means were computed (Table A2; data available at PAGES data repository; see Acknowledgments) using a distance-weighted interpolation of the four neighbored one degree grid points (Program INT3POL, data available through PAGES; see Acknowledgments) to better resolve the effect of oceanographic fronts in regions of high sample density. In comparison with the full  $1 \times 1^\circ$  *Levitus* data set (Figures 1a - 1b), our data set still contains many areas without calibration samples (Figures 6a - 6b). Thus we are still far from an ideal coverage by the calibration data.

### Temperature Estimation Techniques

Mainly two methods of temperature estimation are applied to link the faunal data with SST measurements

The CLIMAP transfer technique [Imbrie and Kipp, 1971; Kipp, 1976] is based on a factor analysis of the species abundance data (the CABFAC routine [see Klován and Imbrie, 1971]), a check for the spatial coherency and oceanographic reliability of the factors, and a stepwise multiple regression procedure to relate quantitatively the end-members of the factor analysis to the "measured" SST. This step has to be repeated until the regression coefficients reach maximum statistical reliability according to the Student-t test. Finally, the results of these two procedures are used by the program "THREAD" (data available at PAGES data repository; see Acknowledgments) to analyse fossil data for the estimation of paleotemperatures.

The modern analog technique [Hutson, 1980] directly measures the difference between the faunal composition of a subject sample with a subset of best analogs of a modern assemblage data set selected by a similarity or dissimilarity index and estimates a temperature as the average or weighted average of the "measured" temperatures at the stations with the best analogs. Several tools of comparison, similarity, or dissimilarity were used [Overpeck et al., 1985].

Both calibration techniques have their advantages and disadvantages [Prell, 1985]: The transfer method as noted by the CLIMAP group [Cline and Hays, 1976; Hutson and Prell, 1980; Prell, 1985; Guiot, 1991] is very sensitive to (1) the selection of the suitable number of factors, (2) the selection of statistically relevant regression parameters, and (3) it also suffers from the

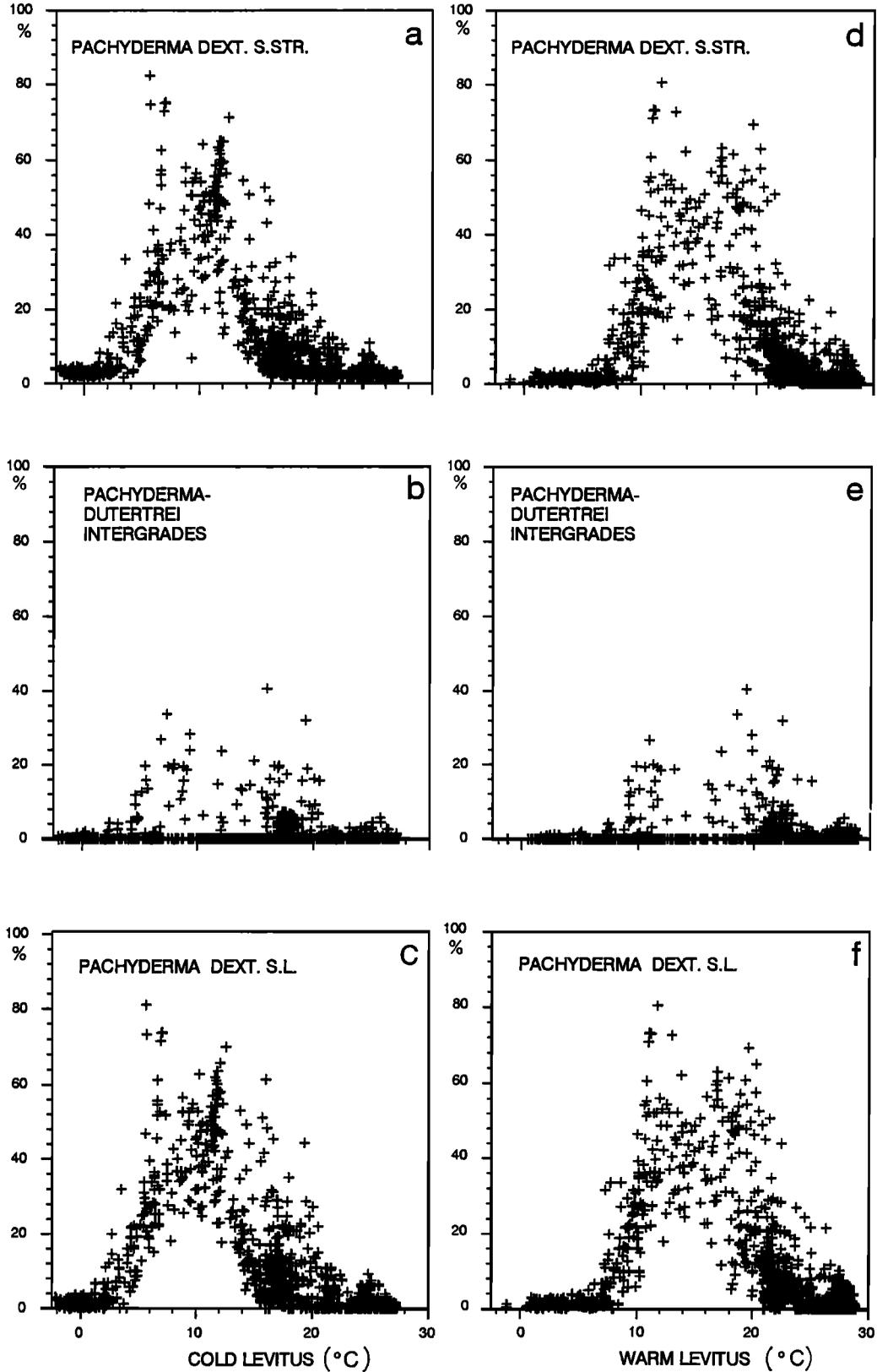
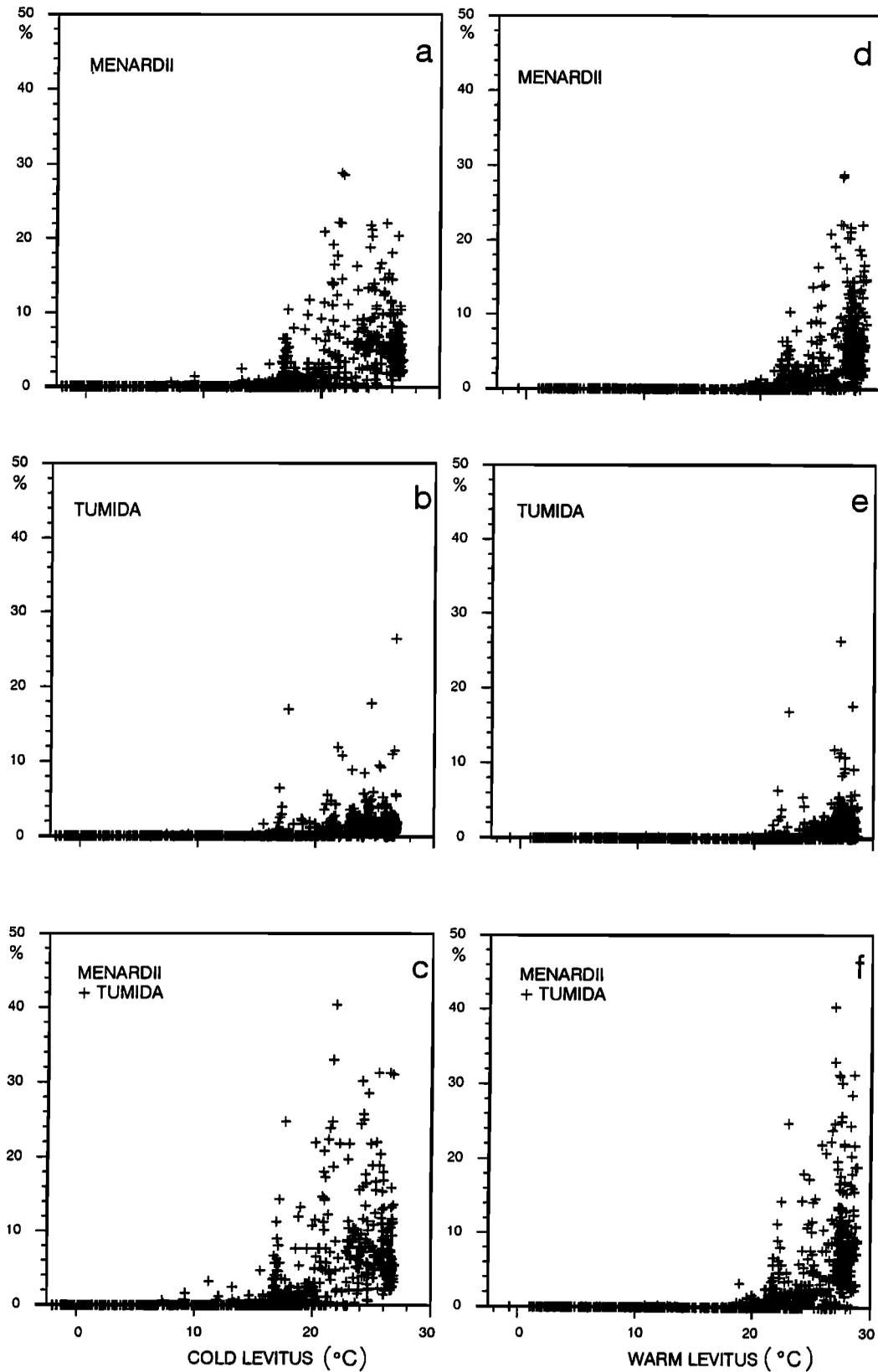
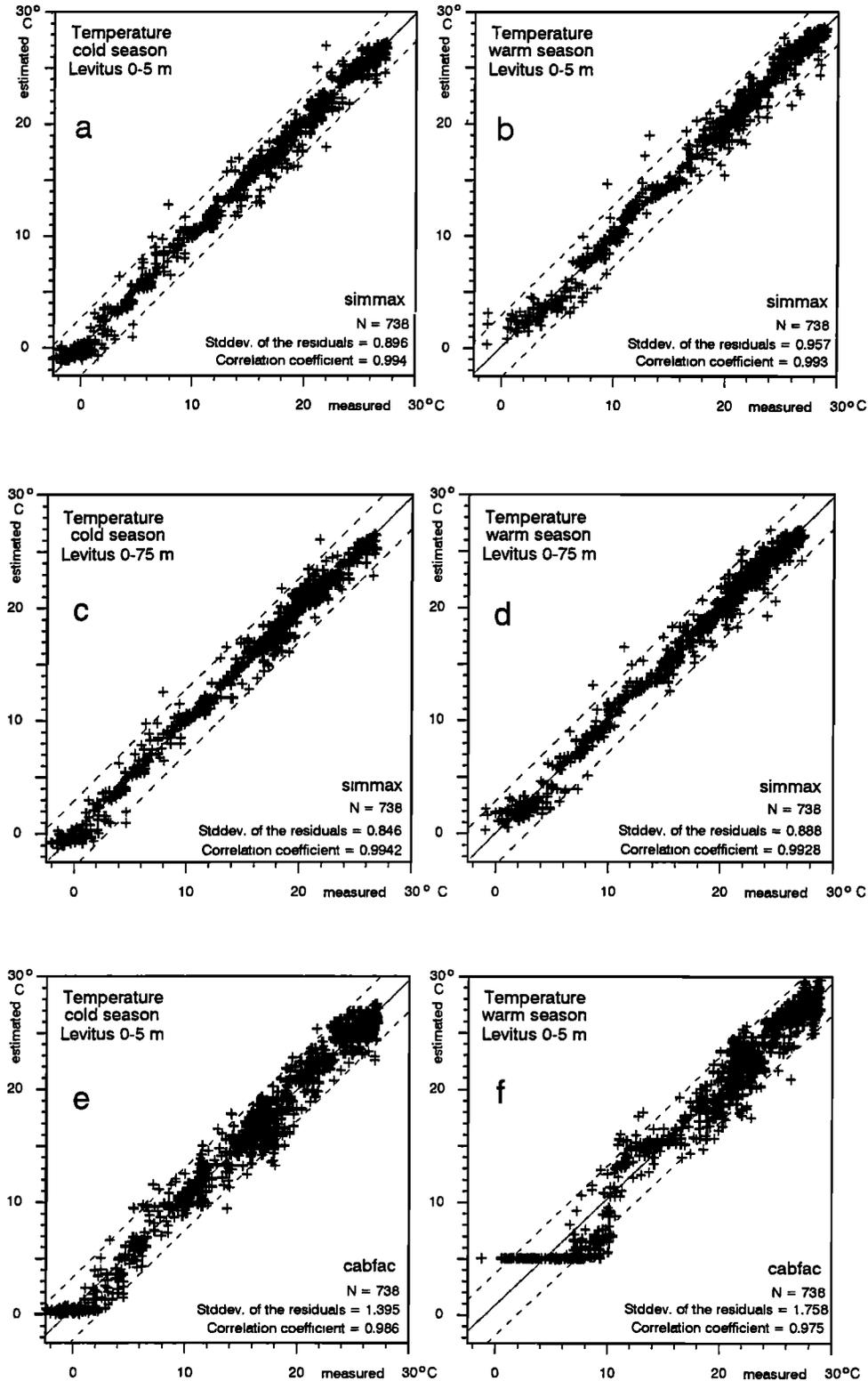


Figure 4. Sea surface temperature preference (x-axis in degrees Celsius) of *Neogloboquadrina pachyderma* var. *dextra s. str.*, the intergrades between *N. dutertrei* and *pachyderma*, and the lumped *N. pachyderma* var. *dextra s. l.* : (a-c) caloric winter temperatures; (d-f) caloric summer temperatures (y-axis is the percentages of total planktonic foraminifera).



**Figure 5.** Sea surface temperature preference of the menardiform globorotalias: caloric winter SST ( $x$ -axis in degrees Celsius) versus (a) *G. menardii*, (b) *G. tumida*, (c) *G. menardii* plus *tumida*; caloric summer SST ( $x$ -axis in degrees Celsius) versus (d) *G. menardii*, (e) *G. tumida*, (f) *G. menardii* +plus *tumida* ( $y$ -axis in percentages of total planktonic foraminifera).



**Figure 6.** Comparison between SIMMAX estimated and measured SST at 0 m (level 1);  $\pm 2^\circ\text{C}$  deviation is indicated for (a) caloric winter, and (b) caloric summer (x and y -axis in degrees Celsius). Comparison between SIMMAX estimated and Levitus measured SST for 0- to 75-m depth, the level showing the best fit for (c) caloric winter and (d) caloric summer. Hatched lines indicate the  $\pm 2^\circ\text{C}$  deviation. Comparison between Climate: Long-Range Investigation, Mapping, and Prediction (CLIMAP) transfer technique-estimated and Levitus [1982] measured temperatures for 0-m (level 1): (e) caloric winter, (f) caloric summer. Hatched lines indicate the  $\pm 2^\circ\text{C}$  deviation.

problem of the restricted number of suitable modern analogs. Samples which have no modern counterpart (no-analog samples) are recognized by the species percentages exceeding the maximum values in the calibration set (Table A1) and are automatically excluded from the analysis to prevent extrapolations into unknown, uncontrolled directions.

The MAT technique simply uses similarities and averages and avoids no-analog situations. It indicates samples with poor analogs within the selected best analogs by a low similarity index. However, with good geographic coverage in the calibration area a reliable average value can be computed. Nevertheless, there is no direct way to evaluate statistically the overall reliability of the results. Therefore each individual estimate must be critically examined by determining the standard deviation of the SSTs of the best analogs and the mean similarity index of the selected most similar samples. Indirectly, the accuracy of the MAT calibration results can be evaluated in terms of the standard deviation of the residuals and the correlation coefficient between the observed and the estimated temperatures.

Regarding the computing efforts, the advantage in applying the CLIMAP transfer technique method is after a time-consuming initial procedure a very quick result from the THREAD routine. The advantage of the MAT technique is that any reliable new sample of the modern fauna can easily be added to the calibration set and then contributes to the result of any subject sample. However, the computational time is prolonged by the square of the number of the input data.

### The SIMMAX Technique

According to the MAT techniques mentioned, the SIMMAX technique searches for a subject sample a predefined number of best analogs of a modern assemblage data set (data available at PAGES data repository; see Acknowledgments) by a similarity index and calculates an estimated SST as an average of the measured modern SST (data available at PAGES data repository; see Acknowledgments) of the stations with those best analogs. It is the weighting of species in the similarity or dissimilarity coefficients that is important in any selection. Following an idea of *Altenbach* [1985] to compare core samples with modern analogs using simple indices and with regard to our initial computer facilities, the scalar product was chosen among the various available [*Overpeck et al.*, 1985]. *Le* [1992] worked on the sensitivities of the CLIMAP transfer function method and the MAT is also pertinent to this point. The square chord dissimilarity coefficient used in MAT [*Prell*, 1985] weights somewhat toward rare species (*J. Le*, personal communication, 1995). Our similarity index used in MAT [*Prell*, 1985] weights somewhat toward rare species (*J. Le*, personal communication, 1995). Our similarity index is simply the scalar product of the (sum of the squared species percentages = unity) normalized assemblage vectors.

$$s_j = \sum_{k=1}^{n_s} \left[ \left( P_k / \sqrt{\text{sum1}} \right) \cdot \left( Q_{j,k} / \sqrt{\text{sum2}} \right) \right] \quad (1)$$

where  $s_j$  is the scalar product of the subject sample and the analog sample  $j$ ,  $n_s$  is the number of species,  $P_k$  is the percentage of the species  $k$  in the subject sample,  $\text{sum1}$  is the sum of the squared percentages of the  $n_s$  species in the subject sample,  $Q_{j,k}$  is the percentage of the species  $k$  in the analog sample  $j$ ,  $\text{sum2}$  is the sum of the squared percentages of the  $n_s$  species in the analog sample  $j$ .

Full similarity is given by a value of 1, and full dissimilarity is given by a value of 0. The scalar product is a measure indepen-

dent of the percentage sum of the components. To study the effect of reduced species categories, we have enlarged the species matrix including the coiling varieties of *G. truncatulinoides* and splitting off the menardiiform complex into *G. menardii cultrata* and *G. tumida* using an extended data set. There was no progress in correlation coefficients using 28 instead of 26 categories. This may be explained by the preference weight given by the scalar product to more abundant species.

The average similarity index is calculated according to formula (2):

$$\text{simmean} = \frac{\sum_{j=j\text{max}(1)}^{j\text{max}(n_n)} (s_j / d_j)}{n_n} \quad (2)$$

where  $\text{simmean}$  is the average similarity index of the subject sample,  $n_n$  is the number of analog samples,  $j\text{max}(k)$  is the array containing the addresses of the  $n_n$  analog samples aligned according to their similarity,  $s_j$  is the scalar product of the subject sample and the analog sample  $j$ , and  $d_j$  is the geographical distance between the subject sample and the analog sample  $j$ .

To define a lower limit of similarity necessary to consider a sample as analog is highly subjective. *Overpeck et al.* [1985] specified potential critical values of several dissimilarity coefficients in pollen analogs but recommended their use with caution. Therefore, along with the estimated SST, the range and standard deviation of the best analogs have to be considered. It is then the responsibility of the interpreter to judge the reliability of the estimates. For orientation, the minimum value of the similarity index in the calibration run is 0.79 (Table 2).

The SST are estimated according to formula (3):

$$t_{\text{est}} = \frac{\sum_{j=j\text{max}(1)}^{j\text{max}(n_n)} (t_j \cdot s_j \cdot d_j^{-1})}{\sum_{j=j\text{max}(1)}^{j\text{max}(n_n)} (s_j \cdot d_j^{-1})} \quad (3)$$

where  $t_{\text{est}}$  is the estimated SST of the subject sample and  $t_j$  is the SST of the object sample  $j$ ; for the other items, see formula (2).

The estimates are scalar product weighted averages of the SSTs of the best analogs weighted by their inverse geographical distance from the location of the subject sample (a "nearest neighbour" weighting). In the calibration set the best analog of a subject sample is itself and has a geographical distance of zero. As the relationships with themselves are redundant, the subject samples are excluded from the search, and this zero distance does not influence the geographical weighting procedure. The procedure to estimate paleo-SSTs from downcore samples therefore also excludes the core-top sample from the core being estimated for the same reason as above. This does have the disadvantage that it excludes possibly a very good candidate from the search. On the other hand, this exclusion of the core-top fauna avoids an exaggeration of the local assemblage by the weighting procedure using near to zero divisors. Samples from the other hemisphere are not excluded by the application of this kind of weighting as there may be good analogs. All (e.g., 10) of the most similar samples selected by the unweighted version of the temperature estimation are included. The procedure of weighting by geographic distance only shifts the power of the nearest neighbors. If the sample coverage on one hemisphere is dense enough and extraordinary faunal changes are not observable, the problem of merely parallel samples from the opposite hemisphere is not crucial for the distance weighting procedure.

**Table 2.** Summary Statistics of SIMMAX Distance-Weighted and Nondistance-Weighted SST Estimates for Winter and Summer

	Similarity Index	Distance Weighted Estimates	Residuals (Measured - Estimated)	Scalar Product Estimates	Residuals (Measured - Estimated)	Minimum SST of Best Analogs	Maximum SST of Best Analogs	Standard Deviation of Best Analogs
<i>SST Cold Season</i>								
Minimum	0.79	-1.40	-5.00	-0.80	-6.00	-2.10	0.30	0.10
Maximum	1.00	27.20	4.00	27.10	5.10	26.80	27.40	5.40
Mean	0.96	14.91	0.05	14.94	0.01	12.95	16.98	1.32
Standard deviation	0.03	8.42	0.90	8.37	1.36	8.42	8.27	0.70
<i>SST Warm Season</i>								
Minimum	0.79	0.40	-5.80	1.60	-7.90	-1.20	4.20	0.10
Maximum	1.00	28.60	4.40	28.50	6.90	28.10	29.00	6.00
Mean	0.96	18.93	0.04	18.94	0.03	16.79	21.11	1.42
Standard deviation	0.03	8.09	0.96	8.02	1.55	8.64	7.57	0.86

A non-distance-weighted estimate is presented as "SST ndw" (data available at PAGES data repository; see Acknowledgments). Except for the larger standard deviations of the residuals and a linear correlation coefficient ( $r = 0.9816$ ) for SSTs of the warm season the statistical data of the SST predictions using the scalar product (Table 3a and 3b) are within the range of the previously mentioned MAT results.

#### Application Procedures of the SIMMAX Technique

For calibration we have applied the SIMMAX technique to 738 input samples (data available at PAGES data repository; see Acknowledgments). The program output contains always along with the average similarity three sets of SST data: (1) regionally distance-weighted temperature estimates, (2) unweighted temperature estimates, and (3) the standard deviations of the unweighted temperature estimates of the best analogs (data avail-

able at PAGES data repository; see Acknowledgments) In the cases of inconsistency, all three values have to be included within the discussion of reliability of the resultant SST estimates.

The inverse geographical distance weighting contributes to a stronger prevalence of regional peculiarities on account that more distant samples have less influence but does not totally suppress ocean-wide relationships. Depending on the samples' geographical position, however, the same faunal composition may result in different paleo-SST estimates. This has advantages in reconstructing the modern situation and a paleoenvironment not too different from the modern one but can be crucial in the case of a strong migration of the fossil faunal provinces away from the modern centers.

The result of the calibration procedure is shown by two scatter diagrams (Figures 6a - 6b) where estimated SST for caloric winter and summer seasons are plotted versus the "measured" atlas values. Considering the number of samples (738), the correlation

**Table 3a.** Results of Modern Analog Technique (MAT) Approaches With the European Project of Oceanic Climate and Hazards (EPOCH) Data Set Using Summary Statistics

	Minimum	Maximum	Points	Standard Deviation of Residuals	Minimum of Residuals	Maximum of Residuals
<i>SST Cold Season</i>						
Euksqu	-0,8	27,1	738	1.21	-5.6	6.0
Eustd	-0,8	27,2	738	1.20	-7.4	6.0
Theta	-0,9	27,1	738	1.21	-5.2	5.1
Chord	-0,9	27,1	738	1.01	-4.9	3.9
Scalar product	-0,8	27,1	738	1.34	-5.2	6.0
Simmax dw	-1,4	27,2	738	0.9	-4.0	5.8
Measured	-2,1	27,4	738			
<i>SST Warm Season</i>						
Euksqu	1,3	28,4	738	1.36	-5.3	8.0
Eustd	1,5	28,5	738	1.30	-7.2	7.9
Theta	1,5	28,5	738	1.38	-6.8	5.1
Chord	1,4	28,5	738	1.09	-5.5	4.4
Scalar product	1,6	28,5	738	1.55	-6.9	7.9
Simmax dw	0,4	28,6	738	0.96	-4.4	5.8
Measured	-1,2	29,0	738			

Abbreviations are euksqu, squared Euklidean distance; eustd, squared Euklidean standard distance; theta, squared cosine theta distance; chord, squared chord distance, simmax dw, SIMMAX geographic distance-weighted; scalar product, SIMMAX non-geographic distance-weighted; measured, *Levitus* [1982] SST, 0-m.

**Table 3b.** Results of MAT Approaches With the EPOCH Data Set Using Linear correlation Parameters to *Levitus* [1982] SST

	Intercept	Increment	Correlation Coefficient
<i>SST cold season</i>			
Eusqu	0,6032	0,9690	0,9858
Eustd	0,2080	0,9811	0,9871
Theta	0,4531	0,9745	0,9854
Chord	0,0989	0,9894	0,9910
Scalar product	0,2740	0,9805	0,9869
Simmax dw	0,1644	0,9893	0,9930
<i>SST warm season</i>			
Eusqu	0,3695	0,9751	0,9897
Eustd	0,0777	0,9864	0,9898
Theta	0,2305	0,9836	0,9897
Chord	0,0717	0,9903	0,9928
Scalar product	0,5385	0,9699	0,9816
Simmax dw	0,0369	0,9942	0,9943

Abbreviations as in Table 3a.

coefficients (>0.99) are extremely high for both seasons, and the standard deviation of the residuals at 0.94°C indicates the high quality of the results though a set of outliers was not removed from the system. A considerable advantage of the SIMMAX technique is gained at the cold end of the data matrix, where it is possible to estimate SST as low as -1.4°C for caloric winter and 0.4°C for caloric summer. These results are crucial for a reconstruction of glacial SSTs in the northern North Atlantic [Weinelt, 1993; Sarnthein *et al.*, 1995], where former approaches failed due to their poor database.

To compare the regional distribution of the SST estimates with the measured, we plotted maps using only the information from the calibration samples (Figures 7a - 7d). The isolines of the estimated and measured SSTs show a very similar pattern. However, due to the partly still incomplete data coverage, there are still differences to the temperature maps constructed by the full Levitus data set (Figures 1a - 1b).

### SST Estimates Obtained by the SIMMAX Technique

The SST estimates obtained by the SIMMAX technique, representing the modern analogs with a standard deviation of 0.9°C for caloric winter residuals and 0.96°C for caloric summer residuals, generally improve the results using previous MAT approaches. According to the standard deviation of the residuals the approach using the scalar products is surely the weakest within the other similarity/dissimilarity indices (see Table 3a). However, regarding the range of the residuals (minimum and maximum deviations), the use of scalar product is not always at the bad end. Anyway, its combination with the geographical distance weighting (the very SIMMAX technique) results in optimal correlation coefficients. Trying MAT with other dissimilarity indices and with distance weighting procedure is investigated.

In detail, the temperature estimates of sample V7-42 for both seasons are >6°C too cold compared with the "measured" ones.

This sample is considered to be of Pleistocene age and was removed from the test data input set despite the fact that there are no other age determinations available.

The linear regression coefficients between Berger's dissolution index and the residuals (Figures A1a and A1b) suggest that the SIMMAX SST estimates are clearly independent of dissolution ( $r = 0.005$  for summer and 0.007 for winter,  $n = 738$ ). As ecological factors as well as dissolution change the species compositions, this independence is not proven. We also did not find systematic biases of the SIMMAX estimates to water depth, which is related to the preservation state. So we confirm the statement that MAT is less plagued by dissolution than the CLIMAP transfer function is [Prell, 1985; J. Le, personal communication, 1995]. Applying the SIMMAX technique to downcore samples (equatorial sediment core 16415, 3841-m water depth, with several severely dissolved sections) [Pflaumann, 1986], the SST estimates are shown to be nearly independent of local preservation as long as the diversity of the fauna does not break down. However, there are some rare samples indicating very low SSTs which cannot be explained by either severe dissolution or by low similarity indices.

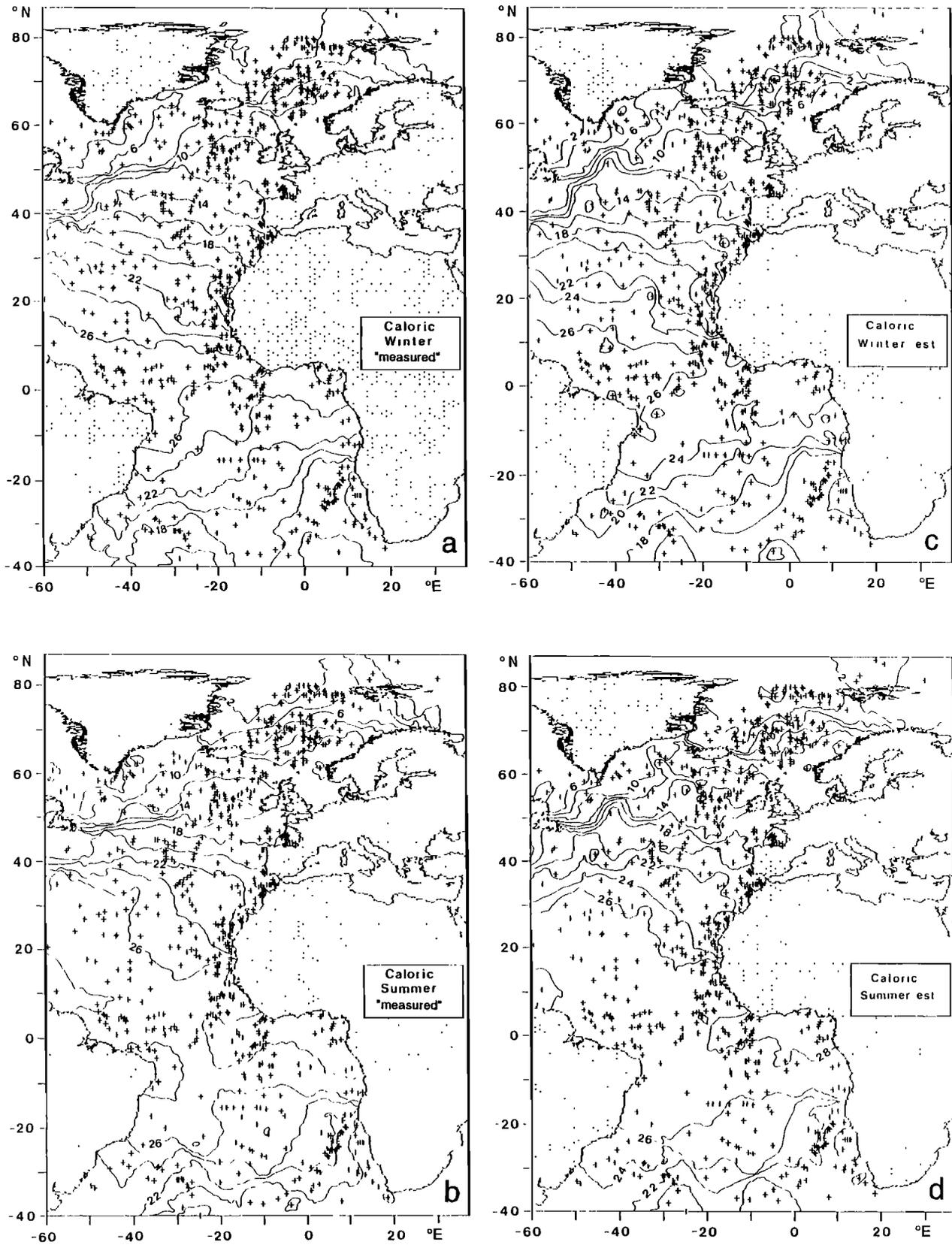
Samples whose estimates deviate by more than 2°C from the measured SSTs are listed in Table A2. Besides SST, no other independent indications are found for these extremes: faunal composition, average similarity index, and standard deviation of the observed temperatures of the 10 best analogs fall well within the range of the data set. Thus samples with high negative residuals (estimated minus measured) in both caloric seasons may be of glacial age, while samples with extremely positive residuals are suspected to be from the Holocene climatic optimum. However, as there are no direct or indirect age determinations available, they were not excluded from the standard input matrix.

### Regional Distribution of the Residuals

The regional distribution pattern of the extreme residuals (Figures A2a and A2b) may help to identify outliers or inconsistencies of the results. Seventeen small spots of outlier samples are common for both caloric winter and summer seasons. Their distribution pattern indicates that six outliers are near the continental margin or on the shelf and that six to seven outliers are at water mass boundaries. As there is no special region with a strong concentration of such outliers, an explanation of these atypical estimates has to be found in their special faunal composition or too strongly smoothed atlas values. We consider the Levitus approach as a sound base for a worldwide temperature distribution pattern; however, it has the problem of being too strongly smoothed in critical regions of oceanic fronts. This also can lead to problems in modelling the proper modern current system by ocean circulation models (D. Seidov, personal communication, 1993).

### Incorporation of Further Water Depth Ranges and Seasons

As the habitat of planktonic foraminifera is not restricted to the very surface layer [Deuser *et al.*, 1981; Ravelo *et al.*, 1990], temperatures of the *Levitus* [1982] defined oceanographic layers 4, 5, and 6 (0, 30, 50, 75 m water depth) as well as the arithmetic means of the temperatures of these deeper layers (layers 1+4, 1+4+5, 1+4+5+6, 4+5, 4+5+6, 5+6) were also used as input parameters for SIMMAX (data available at PAGES data repository; see Acknowledgments) to find which depth range displays the optimum estimates for an ocean wide temperature record. Differences in the linear correlation coefficients between these averages and the estimated temperatures (Table 4a) are very small and might be insignificant. But the trends are remarkable, as 44 independent tests and no change in the sign of the values are hardly to



**Figure 7.** Areal distribution of SST in the Atlantic, derived only by the calibration data: (a) caloric winter SST interpolated from *Levitus* [1982]; (b) caloric summer SST interpolated from *Levitus* [1982]; (c) caloric winter SST estimated by SIMMAX; (d) caloric summer SST estimated by SIMMAX.

**Table 4a.** Summary Statistics of the SIMMAX SST Estimates: Linear Correlation Coefficients for SIMMAX SST Estimates Versus *Levitus* [1882] Data for Four Different Seasons and 738 Samples.

Season	Level	<i>m</i>	1	4	5	6	1+4	1+4+5	1+4+5 +6	4+5	4+5+6	5+6
Cold	1	0	.994*				.994*	)	)			
	4	30		.994*			)	.994*	.994*	.993	)	
	5	50			.992		)	)	)	.993	.992	)
	6	75				.991		)	)	)	)	)
Spring	1	0	.994*				.994*	)	)			
	4	30		.993			)	.994*	.994*	.993	)	
	5	50			.992		)	)	)	.993	.992	)
	6	75				.991		)	)	)	)	)
Warm	1	0	.993*				.993*	)	)			
	4	30		.993*			)	.993*	.993*	.992	)	
	5	50			.991		)	)	)	.992	.991	)
	6	75				.989		)	)	)	)	)
Fall	1	0	.995*				.995*	)	)			
	4	30		.994			)	.995*	.994	.994	)	
	5	50			.992		)	)	)	.993	.991	)
	6	75				.989		)	)	)	)	)

Numbers 1-6 indicate water depth levels of *Levitus* [1982], which are used in various combinations for this correlation test. Here *m* is water depth.

\* The highest correlation coefficients.

be explained by randomness. The highest correlation coefficients are marked by asterisks (Table 4a). Layer 6 (75-m water depth) generally shows the weakest correlations. According to the minimum standard deviation of the residuals (Table 4b), all seasons were best recorded by the mean of all water levels checked (0-75 m). The best results, both with the highest correlation coefficients and relatively low standard deviations, were achieved using the mean of 0- to 75-m water depth for spring temperatures, using the

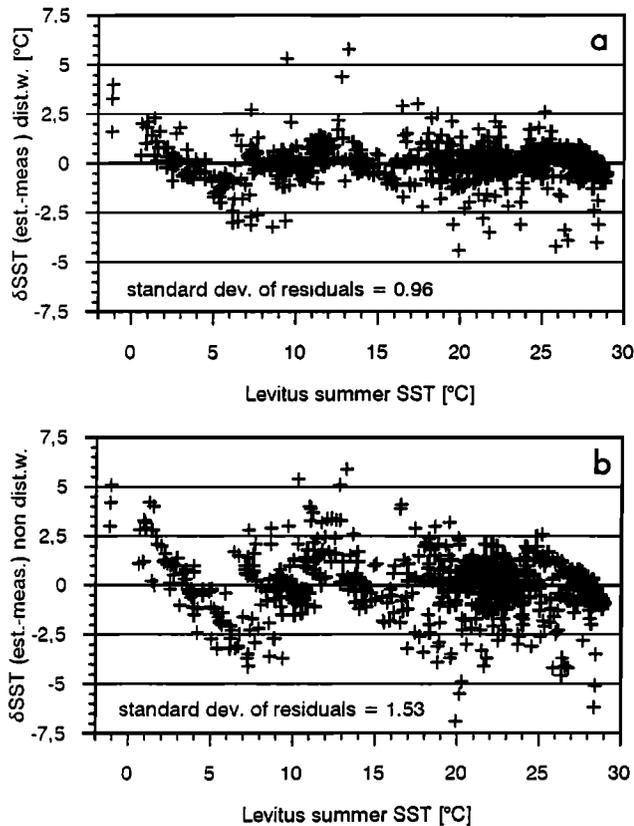
mean of 0- to 50-m water depths for summer and fall temperatures and using the mean of 0- to 30-m water depth for caloric winter temperatures.

These trends in the correlation coefficients and in the standard deviations may indicate that during winter season the temperature relevant species cover a smaller depth range ocean wide than during the other seasons. This can be due either to a weaker temperature sensitivity of the species living in deeper habitats and/or

**Table 4b.** Summary Statistics of the SIMMAX SST Estimates: Standard Deviations for SIMMAX SST Estimates Versus *Levitus* [1882] Data Displayed for Four Different Seasons and 738 Samples

Season	Level	<i>m</i>	1	4	5	6	1+4	1+4+5	1+4+5 +6	4+5	4+5+6	5+6
Cold	1	0	.896				.886	)	)			
	4	30		.918			)	.885	.880*	.927	)	
	5	50			.972		)	)	)	.917	.960	)
	6	75				.986		)	)	)	)	)
Spring	1	0	.913				.882	)	)			
	4	30		.919			)	.861	.847*	.901	)	
	5	50			.939		)	)	)	.888	.926	)
	6	75				.956		)	)	)	)	)
Warm	1	0	.957				.915	)	)			
	4	30		.951			)	.899	.878*	.946	.924	
	5	50			1.000		)	)	)	)	)	.966
	6	75				.975		)	)	)	)	)
Fall	1	0	.854				.855	)	)			
	4	30		.889			)	.851	.850*	.891	)	
	5	50			.945		)	)	)	.892	.945	)
	6	75				.993		)	)	)	)	)

Notations as in Table 4a.



**Figure 8.** Deviation of SIMMAX versus *Levitus* [1982] summer temperatures: (a) distance-weighted estimates; (b) non-distance-weighted estimates.

to a stronger one of the shallow water communities during caloric oceanographic winter. However, during winter the mixed layer is relatively thick [Ravelo *et al.*, 1990], while the production is strongly reduced [Bé *et al.*, 1985; Thunell *et al.*, 1983; Reynolds and Thunell, 1985].

The optimum relations of measured versus estimated SST for caloric winter and summer are presented in the scatter diagrams (Figures 6c and 6d). These observations are corroborated by the regional evaluations of other authors [e.g., Mix *et al.*, 1986; Ravelo *et al.*, 1990] who have studied the influence of the thickness of the mixed layer on the faunal composition.

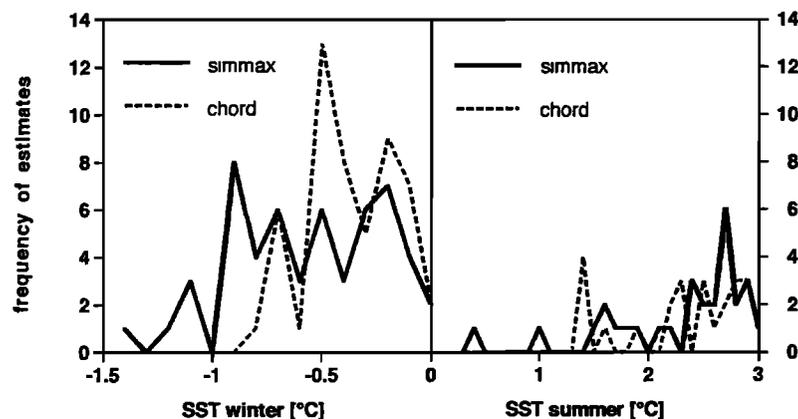
### Limitations of the SIMMAX Technique at the Cold Edge

In fossil glacial samples from high latitudes the left-coiling *N. pachyderma* often is nearly the only planktonic foraminiferal species [Kellogg, 1977; Haake and Pflaumann, 1989; Pflaumann and Hensch, 1994]. In our modern data set (sample 21530) this taxon reaches up to 100% at temperatures of  $-1.2^{\circ}\text{C}$  for winter and  $1.16^{\circ}\text{C}$  for summer (data available at PAGES data repository; see Acknowledgments). However, the extended counts (Figure 2) indicate only a minority of samples containing 100% left-coiling *N. pachyderma*.

As the MAT uses averages of an optional number of best modern analogs, temperature estimates of these extreme samples must be generally too high because there are not enough real modern analogs covering the SST conditions. To analyze the power of the weighting procedure by the geographical distance under these circumstances, we have calculated an artificial sample set at a 2 by 2 degree grid of stations with a faunal composition containing 100% *N. pachyderma* left-coiling variety between  $81^{\circ}$  and  $50^{\circ}\text{N}$  and  $40^{\circ}\text{W}$  and  $30^{\circ}\text{E}$ . The estimated distance-weighted temperatures varied from 0.8 to  $0.3^{\circ}\text{C}$  (from  $-1.9$  to  $-0.6^{\circ}\text{C}$  if the new samples are included) for winter and from 0.5 to  $3.8^{\circ}\text{C}$  (from  $-0.7$  to  $2.4^{\circ}\text{C}$  if the new samples are included) for summer, while the non-distance-weighted estimates are  $0.6^{\circ}\text{C}$  for winter and  $2.1^{\circ}\text{C}$  for summer. The center of the distributional area of the samples with the maximum deviation between the weighted and unweighted estimates for winter is sited off Greenland SW of the Fram Strait and for summer near Jan Mayen.

The deviation of SST estimates, which generally lies near  $\pm 0.96^{\circ}\text{C}$ , is shifting at summer SST of  $>3^{\circ}\text{C}$  to  $+2.5^{\circ}\text{C}$  (for distance-weighted estimates, Figure 8a). This implies that summer SST estimates of less than  $3^{\circ}\text{C}$  are generally too warm. Non-distance-weighted samples are clearly more biased (Figure 8b).

To compare the results of the SIMMAX technique with previous MAT approaches we have fed the ANALOG88 program [Howell, personal communication, 1994] with the actual SIMMAX data set both for analog and subject files and tested all four dissimilarity coefficients: squared cosine-theta distance, squared Euclidean distance, squared standardized Euclidean distance, and squared chord distance. The minimum winter estimates ( $-0.8^{\circ}\text{C}$ ) were calculated using the theta dissimilarity index, while the minimum summer SSTs ( $1.4^{\circ}\text{C}$ ) are computed by the chord method (Table 3a). As the standard error of the SST estimates is virtually the same, the SIMMAX SSTs generated by the geographical weighting procedure were revealed as the best approaches to the measured ones (Figure 9). This is finally cor-



**Figure 9.** Comparison of the SST estimates at the cold end generated by modern analog technique (MAT) with squared chord distance dissimilarity index and by the SIMMAX distance-weighted version.

robored by the linear correlation between estimated and measured SSTs with highest correlation coefficients (Table 3b).

## Results Obtained by the CABFAC/REGRESS Model 738-8-26 as a Concurrent Analytical Method

Our data set was also treated by the CLIMAP transfer technique to achieve a direct comparison of the results. Furthermore, the factor analysis enables us to test the relations of the faunal communities to the oceanographic environment.

### Dimensions of Data and Calculating Parameters

The CLIMAP transfer technique analysis was run on the same data set of 738 samples using the relative abundances of the same 26 species as for SIMMAX (Table A1) with a cutoff at 99% of the variance. Eight factors are statistically relevant within the limits of confidence by the Kaiser criterion [Davies, 1986; Schuchard-Fischer, 1980]. The statistics of the analysis (Table A3) indicate that 96.1% of the variance can be explained by the eight varimax rotated factors. A six-factor model explained only 93.8 % of the variance and underestimated the influence of *Globigerina quinqueloba*, a species common in the subpolar/polar regions with reduced faunal diversity [Bé and Tolderlund, 1971; Kipp, 1976; Ottens, 1992]. This species marks the subpolar front [Pflaumann and Hensch, 1994]. Neglecting the contribution of this species to the model results in reduced communalities for that regions. Samples of low communality whose faunal compositions are not adequately explained by the eight-factor model (Figure A3) are not located in areas where the SIMMAX outliers (Figures A2a and A2b) are found, indicating that this approach depends on species distribution patterns which are different from those applied by the MAT technique.

### Discussion of the End-Members

The following varimax rotated end-members are discussed in order of decreasing amount of sample variance explained by each. The tropical assemblage (Factor 1) is dominated by *Globigerinoides ruber* (white variation) (Table A4) and explains 29% of the variance of the input data (Table A3). The regional distribution of the samples with high factor loadings of this assemblage (Figure A4c) covers the area between 33°N and 35°S, interrupted by some spots of low factor loadings at the equator. A meridional asymmetry of the distributional pattern with low values on the eastern side of the Atlantic can be explained by the influence of the water masses of the northern and southern eastern boundary current systems reaching nearly the caloric equator. A minor spot of high loadings of this factor at 12°S along the African coast is based on two samples with a data gap to the north and west, so its isolation may be of artificial origin.

Scatter diagrams of the factor loadings versus caloric winter and summer temperatures (Figures A4b and A4c) indicate the strong relations between high temperatures and high factor loadings with a strong gradient at 14°-18°C (cold season) and 18°-20°C (warm season). While the cold side has little scatter, there is considerable scatter within the warm temperature regime, which may be explained (1) by the local triggering forces of the tropical upwelling regions, (2) by dissolution, (3) by the fact that faunal variability in the tropical ocean is not a direct function of SST; that is, other surface/near surface water environmental or hydrographic variables could be producing the increased scatter observed in the low latitudes, or (4) by the grid of the Levitus data set being unable to resolve mesoscale patterns.

The cold-intermediate assemblage (Factor 2) is dominated by *Neogloboquadrina pachyderma* var. *dextra* (Table A4), explaining 21% of the variance of the input data set (Table A3). The regional distribution pattern of its major loadings (>0.7) covers at a first glance a somewhat irregular area along the boundary between the North Atlantic Drift and the very cold western boundary currents of the northern hemisphere off Greenland and Labrador (Figure A5a). However, oceanographically, the assemblage delineates water masses of the North Atlantic Drift branching to the northwest (Irminger current), northeast (Norwegian current), and southwest (Portugal current); in addition, there are also isolated areas of high factor loadings of this assemblage within the realm of the Canary current. In the southern hemisphere this assemblage is not as well recorded: to the west around 36°S/30°W it may indicate the northern limit of the Antarctic circumpolar current system, while in the east it outlines the coldest parts of the Benguela current off Southwest Africa. The lower limit of the temperature regime of this factor is 7°-9°C for caloric winter and 9°-11°C for caloric summer with steep slopes at the cold sides and more gentle ones at the warm sides (Figures A5b and A5c).

The polar assemblage (Factor 3) (Figure A6a), is restricted to the northern hemisphere, due to the inclusion of no samples south of 45°S and so excluding the polar realms of the southern hemisphere. It is dominated by left-coiling *Neogloboquadrina pachyderma* (Table A4) and explains 19% of the faunal variation (Table A3). Its distributional pattern covers the main parts of the Greenland-Norwegian Sea and the Labrador Sea. To the south its western boundary is mainly caused by sampling gaps in the Baffin Strait and Denmark Strait, while to the north in the Greenland Sea it is defined by the lack of planktonic forams in the surface sediments caused by low flux rates [Carsten, 1988]. Though overemphasized by the map projection, the extension north and northeast of Svalboard should be noted. Here the eastern boundary of the realm is defined by observational gaps. To the southeast the distribution of the polar assemblage is generally neighbored by the cold intermediate assemblage. With respect to the temperature record the polar assemblage is most abundant below SSTs <5°C for winter and <8°C for summer temperatures (Figures A6b and A6c). The influence of the polar assemblage on the temperature record of the warmer regions (above 8°-10°C) is highly variable especially between 14° and 20°C due to the inability of the low resolution Levitus [1982] data to separate normal warm waters and variable upwelling of cold waters in the subtropics.

The warm-intermediate assemblage (Factor 4) explains 11% of the faunal variance of the input data (Table A3). It is dominated by *Globigerina bulloides* (Table A4) and outlines with high loadings the warmer limits of the cold intermediate assemblage, recording water masses of the inner peripheral parts of the subtropical gyre as well as the upwelling region along the NW African continental margin. The assemblage is similarly distributed in the southern hemisphere though with limited sampling density (Figure A7a). The somewhat scattered distribution between Iceland and Ireland follows the northward directed branch of the North Atlantic Drift and the Irminger current.

Factor loadings are highest at SSTs of 15°C for winter and 21°C for summer with considerable noise especially at the colder temperatures (Figures A7b and A7c). Compared to previously discussed end-members, this factor has only a limited influence on the temperature record. The low noise at winter temperatures above 20°C, however, documents a slight temperature sensitivity.

The subtropical assemblage (Factor 5) is dominated by *Globorotalia inflata* (Table A4). It explains 8% of the variance of the fauna and covers with high negative loadings the subtropical belts of both hemispheres (Figure A8a). Its correlation to temper-

ature is moderate, its peak with the highest (negative) loading being at 16°C during winter and at 22°C during the summer but with clear boundaries to the warm and cold sides, especially excluding temperatures below 10°C (Figures A8b and A8c).

The tropical upwelling assemblage (Factor 6) is dominated by *Neogloboquadrina dutertrei* and the menardiiform globorotalias (Table A4), explaining just 5% of the variance. This assemblage is restricted to the pelagic, noncoastal tropical regions (Figure A9a) along the main oceanic divergencies, and, consequently, the prominent patches of this assemblage are condensed in the eastern part of the Atlantic. However, the scatter diagrams (Figures A9b and A9c) indicate only a weak correlation to temperature.

Factor 7, the equatorial assemblage, contributes only by 1.4 % to the explained variance but helps for the fitting of the model. A six-factor model run with the same data set resulted in a reduced correlation between measured and estimated SST. This assemblage dominated by the *Globigerinoides trilobus* group (Table A4) is regionally restricted to the inner tropical belt, however, in mostly narrow, interrupted belts (Figure A10a). The scatter diagrams (Figures A10b and A10c) indicate that SST alone does not control the factor loadings. The high variance of the factor loadings we explain by the 1° averages of the Levitus data set, too widely spaced for adequately resolving these features.

Factor 8 explains (about 1%) very little of the variance but is important as it contains the remnant variance above the cutoff point defined by the CABFAC procedure. It is dominated by three species: *Globigerina quinqueloba* from subpolar regions and the ubiquitous *Globigerinita glutinata* and *Globigerina falconensis*. Consequently, the regional pattern of its highest loadings is scattered widely (Figure A11a). A pure temperature dependence can be excluded (Figures A11b and A11c), but the assemblage may partly serve as indicator of oceanic fronts.

Except for Factor 1, which is dominated by species sensitive to dissolution, and Factor 3, which is dominated by the dissolution resistant *N. pachyderma*, the preservational bias on the factors can be neglected (Figure A1c).

### Results of the Regression Analysis

These eight factors have been shown to be strongly related to the main surface water masses. This justifies the running of the regression analysis between the factors and the SST.

The multiple regression analysis was run as a nonlinear model of the second degree between the eight factors and caloric winter and summer temperatures of the Levitus level 1 (0-m water depth). Following a suggestion of A. Mix (written communication, 1992), we only allowed terms into the equation that were significant at the 1-alpha = .80 level and left the rest as zero, because they are statistically meaningless. This procedure, however, reduces the quality parameters of the statistics (e.g., SST winter standard error with 44 coefficients = 0.78, with 19 coefficients = 0.88).

**Table 5.** Statistics of Regression Analysis for CABFAC/REGRESS Model 738-8-26

Temperature for Caloric	Winter	Summer
Mean absolute value of residuals	0.9662	1.1143
Standard deviation of absolute value of residuals	0.7870	0.8995
Maximum absolute value	3.7447	4.8342
Minimum absolute value	0.0011	0.0027

Levitus [1982] layer 1 = 0 m. Caloric winter and summer temperatures for 0- to 5-m water depth are given.

**Table 6.** Multiple Regression Coefficients for Model 738-8-26 Regression Equations

Index	Assemblage-Combination	Coefficient	Standard-Error	t -Value
<i>Caloric Winter</i>				
40	F1	20.26647	1.28145	15.815
42	F3	-27.82871	2.22843	-12.488
43	F4	14.42106	0.59216	24.354
36	F5F8	15.94140	1.75333	9.092
23	F2F7	35.30062	2.81363	12.546
16	F1F6	11.86466	0.89176	13.305
22	F2F6	-9.48752	0.69000	-13.750
19	F2F3	13.58088	1.07416	12.643
6	F3SQ	18.62539	2.13412	8.727
14	F1F4	-12.46631	1.24160	-10.041
37	F6F7	22.11730	2.99191	7.392
31	F4F6	5.88384	1.26781	4.641
4	F1SQ	-5.51777	1.15879	-4.762
46	F7	6.53765	0.95172	6.869
32	F4F7	12.52723	1.93951	-6.459
Intercept		10.55128		
<i>Caloric Summer</i>				
42	F3	-29.99808	2.79101	-10.748
40	F1	21.01097	1.76490	11.905
43	F4	25.06242	2.30544	10.871
24	F2F8	-22.41640	1.46655	-15.285
23	F2F7	39.26022	3.80239	10.325
13	F1F3	67.98787	12.14456	5.598
11	F8SQ	23.33327	3.97292	5.873
14	F1F4	-19.15308	2.12675	-9.006
20	F2F4	-12.48354	2.38372	-5.237
7	F4SQ	-12.39228	1.99609	-6.208
4	F1SQ	-10.08904	1.57803	-6.393
19	F2F3	11.29904	1.21456	9.303
6	F3SQ	19.56188	2.67541	7.312
16	F1F6	6.70100	1.02971	6.508
37	F6F7	18.43638	3.44060	5.358
38	F6F8	-5.51424	2.28645	-2.412
10	F7SQ	-6.31219	2.79557	-2.258
Intercept		15.86991		

The statistics of the residuals of this model (Table 5) show patterns similar to those of the SIMMAX technique; however, the standard deviation is somewhat higher. Examining the regression coefficients (Table 6), all the factors contribute to the caloric winter temperatures by their simple loadings but only Factors 1 and 3 by their power loadings. For the caloric summer temperatures the powered loadings of Factors 4, 7, and 8 are also important.

### Discussion of the SST Estimates Obtained by the CABFAC/REGRESS Procedure

The diagrams "estimated versus measured SST" (Figures 6e and 6f) show very high correlation coefficients ( $r = 0.98$  for winter,  $r = 0.97$  for summer,  $n = 738$ ), however, not as high as that of the SIMMAX technique (Figures 6a and 6b). There is, especially for the summer season, considerable noise at the cold edge, where the estimates end at about 5°C for summer and 0.8°C for winter.

The regional distribution patterns of the maximum deviations (>4°C) between estimated and measured SST (Figures A2b and A2d) in some cases are similar to those of the SIMMAX technique, indicating common problems (e.g., east of the Cape of

Good Hope and east off Cape Sao Roque). For the caloric winter season, samples with large residuals (in both directions) are arranged along the margins of the dominant temperature controlled factors, i.e., along the Greenland current, the Norwegian shelf, and on both sides of the North Atlantic Drift. Another area, comparably less densely sampled, is sited within the southern subtropical convergence zone.

The large summer season residuals (Figure A2d) have a distribution pattern similar to the winter ones (Figure A2b). Additionally, they show a poor resolution for the polar region north of Svalboard and in the Labrador Sea.

Despite overall high linear correlation coefficients (Figures 6e and f) and a standard deviation of about  $1.5^{\circ}\text{C}$  (Table 5), the results of the regression procedure are poor for polar regions, because of a lack of surface samples in these areas. The unsatisfactory results may also be caused by calibrating the model for a wide study area so that it is not possible to model particular regional variations.

## Discussion

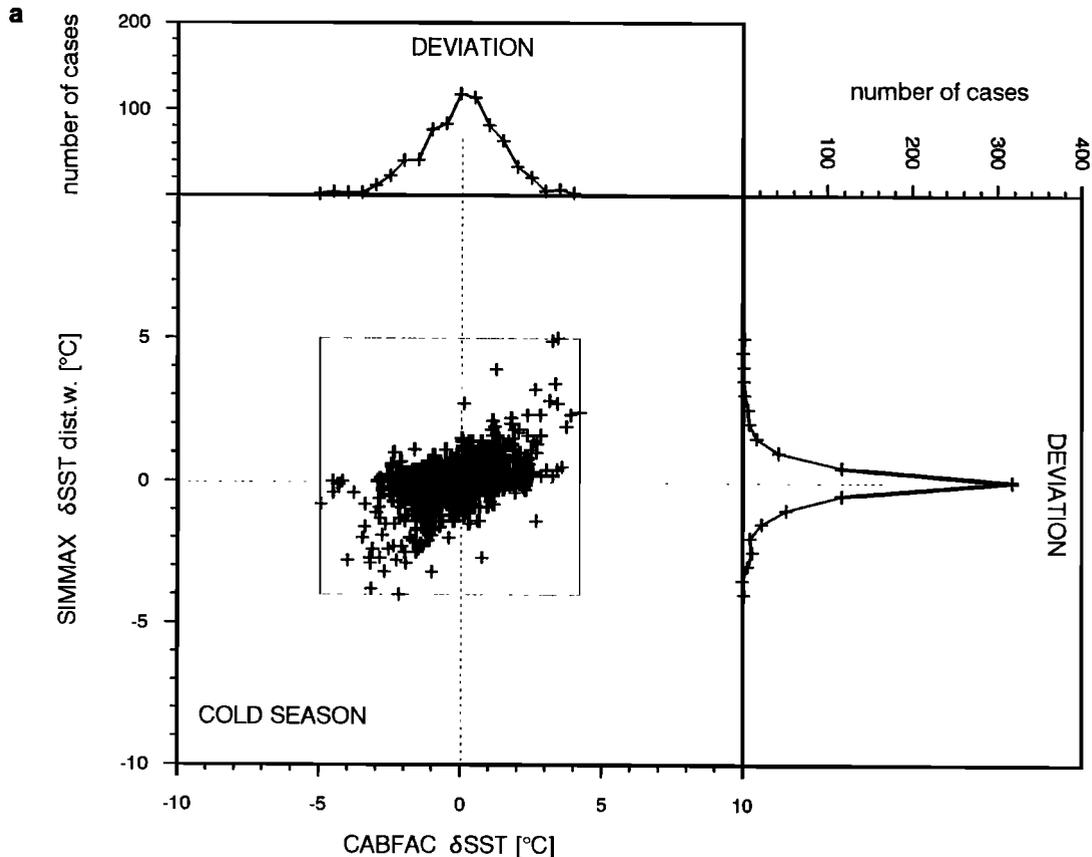
The deviations between measured and estimated SST of CLIMAP and SIMMAX methods (Figures 10a and 10b) have a similar range, indicating that results from both techniques differ only in details. However, the frequency distributions of the SIMMAX residuals have a distinctly higher and narrower maximum around zero, as indicated by the correlation coefficients and

the standard deviations for both caloric winter and summer temperatures. In cases when the SIMMAX technique indicates "unreasonable" high temperatures, we consider the lowest temperature estimate, either weighted or unweighted, as most reliable. For extremely cold paleoenvironments the modern data set is still too small; more investigations at very cold sites are in progress.

The SIMMAX technique using planktonic foraminiferal assemblage data to estimate paleo-SSTs in the whole eastern Atlantic has been successfully applied and shows excellent calibration results comparing measured and estimated data for modern time. However, more densely spaced SST data are needed in regions with strong temperature gradients to obtain a better resolution for the reconstruction of oceanographic fronts.

## Conclusions

1. The reliability of paleotemperature estimates has been significantly improved using a set of 738 samples of planktonic foraminiferal percentage data compiled from the Atlantic between  $40^{\circ}\text{S}$  and  $87^{\circ}\text{N}$  and east of  $60^{\circ}\text{W}$ . New samples originate especially from the continental margins and the Nordic Seas. To include data of workers who did not separate all taxa considered in our data set, we reduced it to 26 categories. Seasonal caloric temperatures from 0-, 30-, 50-, and 75-m water depth at each site were interpolated from the worldwide homogenous data set of Levitus [1982].



**Figure 10.** Comparison of SST deviations (in degrees Celsius) from Levitus [1982] data set, as derived from SIMMAX and CLIMAP transfer technique (model 738-8-26) at 0-m water depth: (a) caloric winter; (b) caloric summer. Frequency distribution of SIMMAX deviation values is clearly more focussed to zero than the distribution of CLIMAP transfer technique values.

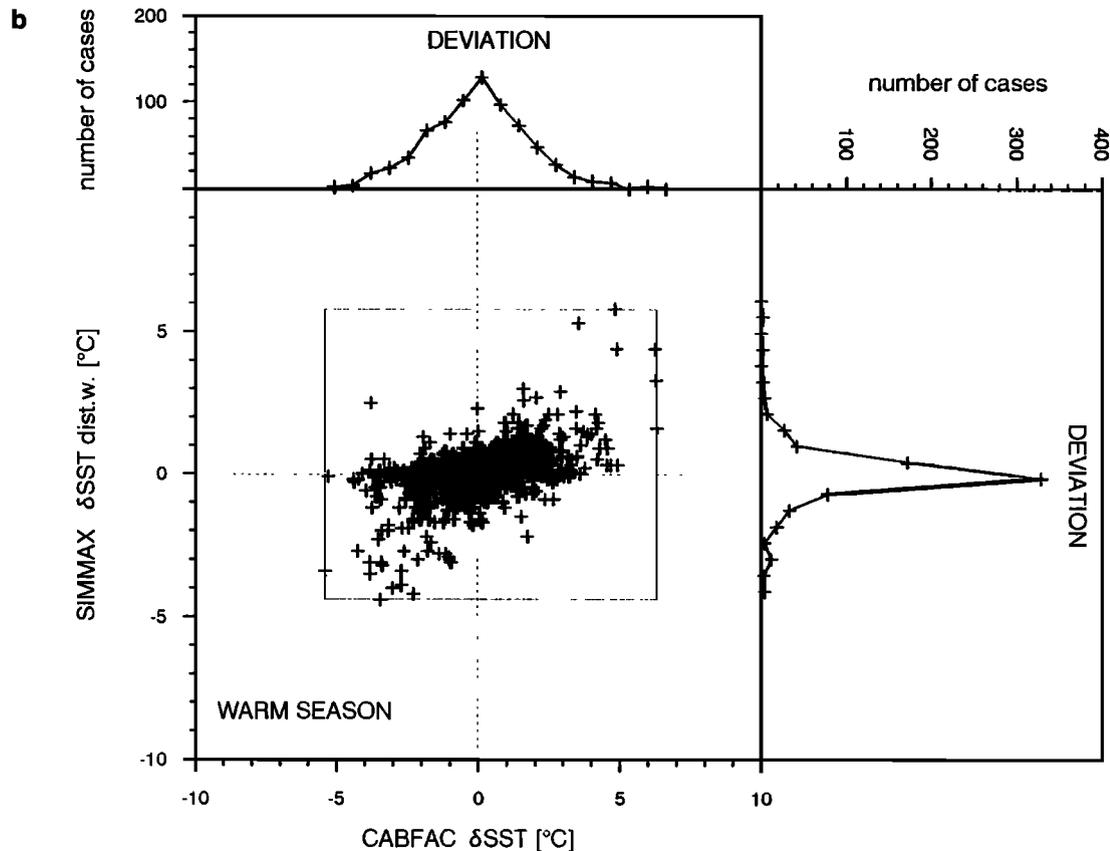


Figure 10. (continued)

2. Reliable results for sea surface temperature (SST) estimates by the modern analog technique (MAT) were obtained using the scalar product of the normalized faunal percentages as similarity index. The average of the SSTs of the 10 best analogs, weighted by the scalar product, was used as estimate of the subject sample. The linear correlation coefficient between the 738 estimates and measured SSTs is 0.987 for the cold and 0.982 for the warm season.

3. The subsequent weighting of the best analogs by their inverse geographical distance from the subject sample site raised the correlation coefficient to 0.994 for the SST of caloric winter and to 0.993 for caloric summer for both 0 m and the average of 0- to 75-m water depth. The standard deviation of the residuals is 0.90° for caloric winter SST and 0.96° for caloric summer SST at 0-m water depth and 0.88° for both caloric winter and summer for the average of the water column between 0- and 75-m water depth. The weighting by the geographical distance takes care of regional peculiarities in the SST estimates.

4. Among various approaches with the MAT the SIMMAX technique is the most straightforward approach in estimating SSTs from planktonic foraminiferal assemblages of the seafloor. As a MAT method it is fairly insensitive to dissolution problems.

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