

Efficacy of $\delta^{18}\text{O}$ data from Pliocene planktonic foraminifer calcite for spatial sea surface temperature reconstruction: comparison with a fully coupled ocean–atmosphere GCM and fossil assemblage data for the mid-Pliocene

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Abstract – Sea surface temperature (SST) estimates using the $\delta^{18}\text{O}$ composition of fossil planktonic foraminifer calcite, within the time slice 3.12 to 3.05 Ma (Pliocene, Kaena Subchron – C2An1r) are assessed for nine Atlantic Ocean sites. These are compared with SST estimates from fossil assemblages for the ‘Time Slab’ 3.29–2.97 Ma and with estimates from a fully coupled ocean–atmosphere General Circulation Model (GCM) for the same time interval. Most SST estimates derived from the $\delta^{18}\text{O}$ data indicate a cooler ocean surface than at present, through the latitudinal range 69.25° N to 46.88° S. At some sites the temperature difference is greater than 5 °C (cooler than at present). This contrasts with SST estimates from fossil assemblages that give warmer than present temperatures at mid- to high latitudes, and similar temperatures in the tropics, and with the GCM, which predicts SSTs warmer than at present across all latitudes for this time interval. Difficulties interpreting the ecology of fossil foraminifer assemblages and inaccurate estimates of mid-Pliocene seawater $\delta^{18}\text{O}$ composition ($\delta^{18}\text{O}_{\text{sw}}$) at some sites may partly produce the temperature discrepancy between isotope-based and fossil-based SST estimates, but do not adequately explain the cool signal of the former. We interpret the cool SST estimates from the $\delta^{18}\text{O}$ data to be the product of: (a) calcite formed at a level deep within or below the ocean mixed-layer during the life-cycle of the foraminifera; (b) secondary calcite with higher $\delta^{18}\text{O}$ formed in the planktonic foraminifer tests in sea bottom pore waters. Although these effects differ between sites, secular and temporal oceanographic trends are preserved in the primary calcite formed in the mixed-layer near the ocean surface, witnessed by the latitudinal variation in estimated SSTs. Reconstructing accurate mid-Pliocene SSTs with much of the existing published oxygen isotope data probably requires a detailed re-assessment of taphonomy, particularly at tropical sites. This study also indicates that methods for estimating Atlantic Pliocene $\delta^{18}\text{O}_{\text{sw}}$ need to be refined.

Keywords: Pliocene, foraminifer, oxygen isotopes, diagenesis.

1. Introduction

Sea surface temperatures (SST) are a key component of global datasets used for driving and validating General Circulation Models for climate (Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999). SSTs are estimated by a variety of means, including fossil assemblages (e.g. Dowsett, Barron & Poore, 1996), alkenone unsaturation analysis (e.g. Herbert & Schuffert, 1998; Haywood *et al.* 2005) and the oxygen isotope composition of the calcite tests of surface dwelling and near-surface dwelling planktonic foraminifera (Erez & Luz, 1983; Bemis *et al.* 1998; Mulitza *et al.* 2003; Spero *et al.* 2003). The efficacy of all of these techniques is debated (e.g. for alkenones see Bijma *et al.* 2001), particularly the oxygen isotope technique for producing absolute

estimates of SSTs in fossil assemblages (Schrag, DePaolo & Richter, 1995; D’Hondt & Arthur, 1996; Pearson *et al.* 2001; Pearson, Ditchfield & Shackleton, 2002; Norris *et al.* 2002; Zachos *et al.* 2002; Williams *et al.* in press and references therein), though all authors concur that the technique is useful for identifying secular and temporal changes in oceanography.

In this paper we analyse published oxygen isotopic records from planktonic foraminifer tests at nine sites in the Atlantic Ocean, within the interval of the Kaena Subchron (3.12 to 3.05 Ma). This time-slice is characterized by a number of chronological events that can be readily correlated (Fig. 1). During the Kaena Subchron the oxygen isotope record from benthic foraminifera suggests global ice volumes generally less than at present, or briefly about the same (Shackleton *et al.* 1995), indicating a generally warmer world (Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999).

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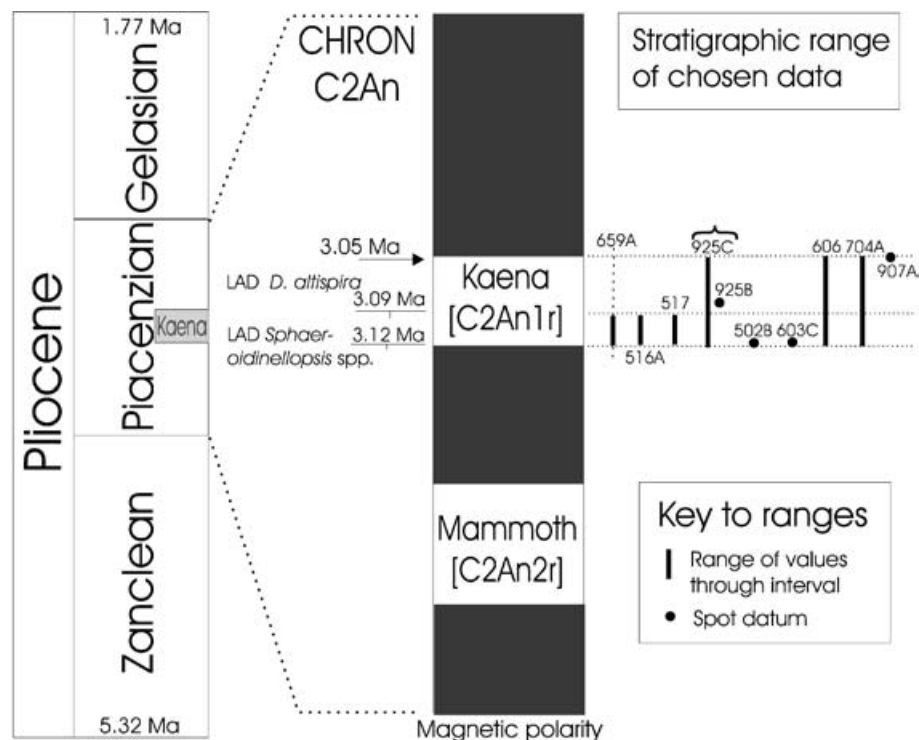


Figure 1. Chronology of nine Atlantic sequences within the interval of the Kaena Subchron. At DSDP sites 516A and 517 and ODP Hole 659A, chronology is based on the LO (last occurrence datum) of *Sphaeroidinellopsis* sp. (3.12 Ma) and the LO of *Dentoglobigerina altispira* (3.09 Ma). At ODP Hole 925B, the isotope datum given by Chaisson & Ravelo (1997) is correlated by means of astrochronology, supported by the LO of *D. altispira* at 90.09–90.66 mbsf (in Hole 925B). For Hole 925C, chronology is based on the age model of Franz (1999; see also Tiedemann & Franz, 1997). At sites/holes 502B, 603C, 606, 704A and 907A the interval is tied with the magnetostratigraphy (for source references, see Fig. 3a,b and main body of the text), though the resolution is poorer at DSDP Site 606 (Keigwin, 1987). The LO of *D. altispira* at about 72.35 m at DSDP site 502B is an additional datum which indicates the Kaena Subchron. Some of the biochronological data used in the reconstruction of this figure is sourced from the Ocean Drilling Stratigraphical Network (data resource at the Leibniz-Institut für Meereswissenschaften at the University of Kiel, IFM-GEOMAR); see the website: <http://www.odsn.de/odsn/services/rangecharts/rangecharts.html>

Analysis of the oxygen isotope signature of bulk carbonates has identified relatively constant SSTs in the tropics through the Tertiary (Schrag, DePaolo & Richter, 1995). Pearson *et al.* (2001) have contrasted the globally warm Late Cretaceous–Early Tertiary ‘Greenhouse’ climate with cool SST estimates for the tropics (15–23 °C) from oxygen isotope palaeothermometry of planktonic foraminifer tests of the same age. They explained this temperature discrepancy in terms of the widespread precipitation of early diagenetic calcite, with higher $\delta^{18}\text{O}$, in planktonic foraminifer tests in sea bottom pore waters. We examine this hypothesis by reference to the mid-Pliocene (3.29 to 2.97 Ma), the last period in geological history when atmospheric CO_2 concentrations were the same as modern (Raymo *et al.* 1996). It was a period of sustained global warmth spanning 300 000 years (e.g. Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999; Haywood, Valdes & Sellwood, 2000). Fossil assemblage data from the mid-Pliocene analysed by the PRISM Group (Pliocene Research, Interpretation, and Synoptic Mapping) indicate SSTs warmer at mid- to high latitudes during this interval, and largely unchanged in the tropics. Some of the sites studied by

PRISM also yield oxygen isotope data from planktonic foraminifer tests. In this paper we examine the efficacy of this published isotope data for spatial reconstruction of Pliocene SSTs, comparing the temperature estimates with those made by PRISM, and with those from a fully coupled ocean–atmosphere GCM for the mid-Pliocene.

2. Dataset and methodology

2.a. Stratigraphy, definitions and data

The mid-Pliocene ‘Time Slab’ was defined by the PRISM Group as that interval between 3.29 and 2.97 Ma, lying between the transition of oxygen isotope stages M2/M1 and G19/G18 (Shackleton *et al.* 1995), in the middle part of the Gauss Normal Polarity Chron (Dowsett *et al.* 1999). The ‘Time Slab’ represents a climatically distinct period during Pliocene times when Earth’s climate was, on the whole, warmer than at present (Dowsett *et al.* 1999). The PRISM group constructed a global dataset of fossil assemblages from 77 marine sites (foraminifera, ostracods, diatoms) that were used to reconstruct sea temperatures and oceanography for the mid-Pliocene (e.g. Dowsett,

Barron & Poore, 1996; Dowsett *et al.* 1999). SSTs were estimated from fossil assemblages of surface-dwelling planktonic foraminifera (e.g. Dowsett & Poore, 1991) and diatoms (e.g. Barron, 1995, 1996). PRISM observed increased SST at mid- and high latitudes in both hemispheres, and little or unchanged SST conditions at low latitudes. This was interpreted as enhanced meridional ocean heat transport (Dowsett *et al.* 1992). Warming was most pronounced in the northeast North Atlantic (Dowsett *et al.* 1999), thought to represent an enhanced Gulf Stream. Data from alkenone palaeothermometry and from a recent modelling study (Haywood & Valdes, 2004; Haywood *et al.* 2005) suggest that low-latitude sea surfaces may also have been warmer than at present, a pattern that could be expected as a result of higher concentration of atmospheric CO₂, which would act to warm the oceans globally.

The Kaena Subchron (C2An1r) is the interval from 3.12 to 3.05 Ma within the Gauss Normal Polarity Chron. It is associated with a number of biochronological events that define the *Sphaeroidinellopsis seminulina*–*Dentoglobigerina altispira* planktonic foraminifera Zone (PL4), which has an estimated range of 3.12–3.09 Ma (Berggren *et al.* 1995; Fig. 1). The base of the interval equates to the last appearance datum (LAD) of *Sphaeroidinellopsis* spp. (Weaver & Clement, 1987). The LAD of *Dentoglobigerina altispira* occurs at 3.09 Ma. The top of the Kaena Subchron has an estimated age of about 3.05 Ma (see Berggren *et al.* 1995; Fronval & Jansen, 1996). Oxygen isotope stage G22 lies towards the top of this interval (Shackleton *et al.* 1995).

The dataset analysed here is from nine Deep Sea Drilling Project/Ocean Drilling Program (DSDP/ODP) sites/holes in the Atlantic Ocean that preserve oxygen isotope data from planktonic foraminifer calcite within the interval of the Kaena Subchron (Figs 1–3). Although the number of Atlantic sites is small, and limited to those with precise chronology for the Kaena Subchron, they nevertheless span a modern latitudinal range of 69.25° N to 46.88° S, covering a wide range of modern SSTs (5.3 to 27.6°C). The data vary from a single oxygen isotope value at some sites, to 18 isotopic values through this interval at ODP Hole 925C (Fig. 4). Six different foraminifer species are used for the Atlantic SST estimates, requiring five different temperature equations (Fig. 5). Modern SST variation is based on Reynolds & Smith (1995) and Smith & Reynolds (1998) who integrated *in situ* (ship and buoy) SST data, satellite retrievals and sea-ice coverage data to produce a 1° spatial resolution monthly climatology (dataset available at http://www.emc.ncep.noaa.gov/research/cmb/sst_analysis).

2.b. Assessing the oxygen isotopic composition of seawater

A key variable required for palaeotemperature calculation is the isotopic composition of the seawater ($\delta^{18}\text{O}_{\text{sw}}$)

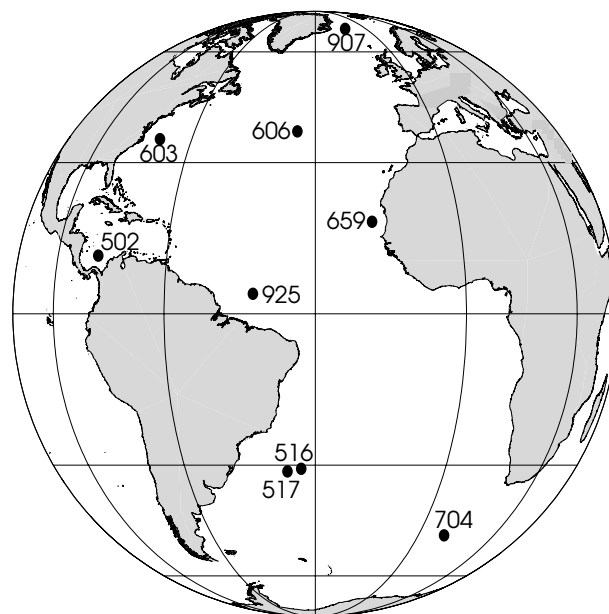


Figure 2. Palaeolatitudinal distribution of nine marine sequences with oxygen isotope data from planktonic foraminifera for the Kaena Subchron interval in the Atlantic Ocean, plotted onto a mid-Pliocene (at 3.5 Ma) reconstruction of geography (courtesy of Dr Roy Livermore, BAS).

in which the foraminifer grew. On a timescale of less than 10 million years, the global mean oxygen isotopic composition of seawater is dependent primarily on the volume of continental ice-sheets (Bice, Sloan & Barron, 2000). At times of ice-sheet presence, such ice acts as an effective reservoir for the lighter oxygen isotope ¹⁶O, resulting in elevated (more positive) $\delta^{18}\text{O}$ levels in the world's oceans. Shackleton & Kennett (1975) estimated that for time periods of ice-free conditions, such as the Cretaceous and Early Cenozoic, the mean seawater composition would have been approximately -1.0‰ Standard Mean Oceanic Water (SMOW); present ice-volumes give $\delta^{18}\text{O}_{\text{sw}}$ of 0.0‰ SMOW. The ice-free value has been applied to studies of the oceans of the Early Tertiary (Zachos, Stott & Lohmann, 1994; Bice, Sloan & Barron, 2000) but is unsuitable for calculations of the mid-Pliocene, as there is good evidence for the presence of continental ice, though the Antarctic Ice Sheet may have been one third smaller (Webb *et al.* 1984; see also Lear, Elderfield & Wilson, 2000). Thus, we add a correction factor for $\delta^{18}\text{O}_{\text{sw}}$ of -0.33‰ SMOW in some of our calculations (Fig. 4).

The local or regional oxygen isotopic composition of surface seawater $\delta^{18}\text{O}$ ($\delta^{18}\text{O}_{\text{sw}}$) is a function of the global mean composition as well as geographical variations caused by the combined effects of changes in evaporation–precipitation patterns, runoff (in coastal regions), and ocean circulation patterns (Zachos, Stott & Lohmann, 1994; Schmidt, 1998). We have used three different methods to assess regional $\delta^{18}\text{O}_{\text{sw}}$.

a)

ODP/ DSDP Site	Foraminifer species	Palaeolat. (modern in brackets)	Palaeolong. (modern in brackets)	Location	Core depth interval for Kaena Subchron	Wolf-Welling, Brenner, Mienert & Thiede (1997) age/depth model
907A	<i>pachyderma</i> (sin)	69.5 (69.25)	-11.98 (-12.7)	Iceland Plateau	depth 57.95mbsf	
606	<i>bulloides</i>	37.6 (37.34)	-34.02 (-35.5)	W flank, Mid Atlantic Ridge	depth 94.28 to 100.25m	90-117mbsf = 3 to 3.5 Ma
603C	<i>ruber</i>	35.84 (35.49)	-68.7 (-70.03)	continental rise, E of N Carolina	core 15,CC (depth ca. 120m)	110-170mbsf = 3 to 3.5 Ma
603C	<i>obliquus</i>	35.84 (35.49)	-68.7 (-70.03)	continental rise, E of N Carolina	core 15,CC (depth ca. 120m)	110-170mbsf = 3 to 3.5 Ma
659A*	<i>sacculifer</i>	18.42 (18.08)	-20.43 (-21.03)	Cape Verde Ridge, off W Africa	cores 10H-1, 26-30 to 10H-4, 140-142 (depth 84.08-89.68m)	85-100mbsf = 3 to 3.5 Ma
502B	<i>quadrilobatus</i>	11.76 (11.48)	-78.45 (-79.38)	Colombia Basin, Caribbean	core 18,CC, depth 76.41m	
925B	<i>sacculifer</i>	4.55 (4.12)	-41.88 (-43.3)	Ceara Rise	core 10H-6, 65-67, depth 88.65mbsf	
925C	<i>sacculifer</i>	4.55 (4.12)	-41.88 (-43.3)	Ceara Rise	composite depths 97.29 to 98.99m	
516A	<i>sacculifer</i>	-29.82 (-30.28)	-33.72 (-35.28)	Rio Grande Ridge	core 4-1 to core 4-2 (depth ca. 12-15m)	11-12mbsf = 3 to 3.5 Ma
516A*	<i>sacculifer</i>	-29.82 (-30.28)	-33.72 (-35.28)	Rio Grande Ridge	core 3-3, within depth 11-12m	11-12mbsf = 3 to 3.5 Ma
517	<i>sacculifer</i>	-30.48 (-30.93)	-36.45 (-38.03)	Rio Grande Ridge	core 10-2 to core 12-1 (depth ca. 39 to 46m)	39.5-43mbsf = 3 to 3.5 Ma
704A	<i>bulloides</i>	-46.76 (-46.88)	7.37 (7.42)	South Atlantic	cores 19-6, 1-5 to 19-7, 18-22 (comp. depth 169.2-171.2m; for real depth add 6.7m)	175-185mbsf = 3 to 3.5 Ma
704A	<i>pachyderma</i> (sin)	-46.76 (-46.88)	7.37 (7.42)	South Atlantic	cores 19-6, 1-5 to 19-7, 18-22 (comp. depth 169.2-171.2m; for real depth add 6.7m)	175-185mbsf = 3 to 3.5 Ma

b)

ODP/ DSDP Site	Foraminifer species	Lithology	Material	Primary reference
907A	<i>pachyderma</i> (sin.)	silt and clay		Fronval & Jansen, 1996
606	<i>bulloides</i>	calcareous ooze	size fraction 180-300 micron	Keigwin, 1987
603C	<i>ruber</i>	calcareous clay	5-20 specimens, above 160 micron (dissolution)	Ganssen, 1987
603C	<i>obliquus</i>	calcareous clay	5-20 specimens, above 160 micron (dissolution)	Ganssen, 1987
659A*	<i>sacculifer</i>	nannofossil ooze		Tiedemann, 1991
502B	<i>quadrilobatus</i>	calcareous marl	size fraction 175-295 micron	Keigwin, 1982a, 1982b
925B	<i>sacculifer</i>	nannofossil ooze (some clay)	6-10 non-saccate specimens, size 355-425 micron	Chaisson & Ravelo, 1997
925C	<i>sacculifer</i>	nannofossil ooze (some clay)		Franz, 1999
516A	<i>sacculifer</i>	calcareous ooze	non-saccate specimens (300-355 micron) (small)	Leonard, Williams & Thunell, 1983
516A*	<i>sacculifer</i>	calcareous ooze	non-saccate specimens (300-355 micron) (small)	Leonard, Williams & Thunell, 1983
517	<i>sacculifer</i>	calcareous ooze	non-saccate specimens (300-355 micron) (small)	Leonard, Williams & Thunell, 1983
704A	<i>bulloides</i>	siliceous & calcareous oozes	size fraction 212-295 micron	Hodell & Venz, 1992
704A	<i>pachyderma</i> (sin.)	siliceous & calcareous oozes		Warnke, Marzo & Hodell, 1996

Figure 3. (a,b) Planktonic foraminifera and DSDP/ODP sites used to evaluate SSTs for the Kaena Subchron. The range of data at ODP Site 659A may encompass levels above and below the Kaena Subchron. Palaeolatitude and palaeolongitude (a) are calculated from a mid-Pliocene (at 3.5 Ma) palaeogeographic reconstruction courtesy of Dr. Roy Livermore (BAS). Also included is the age–depth model (a) of T. C. W. Wolf-Welling, W. Brenner, J. Mienert & J. Thiede, 1997, SYNATLAN-database biochronostratigraphy of Atlantic DSDP/ODP drill sites, available via the Leibniz-Institut für Meereswissenschaften at the University of Kiel (IFM-GEOMAR): <http://www.geomar.de/~twolf/ListADModels.html>. This is based on graphic correlation of 155 ODP and DSDP sites in the Atlantic. In general, this age model concurs with the depths for the 3.05 to 3.12 Ma time interval determined by conventional chronological means, though the age/depth relationship at Hole 516A is slightly different. For this reason, we also calculate isotopic values between depths 11–12 m at this site (core 3–3), denoted as 516A* in the figure.

Zachos, Stott & Lohmann (1994) proposed an equation relating $\delta^{18}\text{O}_{\text{sw}}$ to palaeolatitude. Using present-day open ocean data collected as part of the Geochemical Ocean Sections Study (GEOSECS), they derived the

following equation:

$$\delta^{18}\text{O}_{\text{sw}} = 0.576 + 0.041y - 0.0017y^2 + 1.35 \times 10^{-5}y^3 \quad (6)$$

ODP/ DSDP Site and foram. species	Foraminifer calcite - $\delta^{18}\text{O}$ [VPDB], for Kaena subchron interval (3.12Ma to 3.05Ma)	Present estimate $\delta^{18}\text{O}_{\text{sw}}$ [SMOW] (model Xajpa)	Estimated Local $\delta^{18}\text{O}_{\text{sw}}$ [SMOW] for the mid Pliocene				Estimated Mean SST					Present mean annual temperature	SST estimates from coupled model xatsb	PRISM2 SST mean annual (<i>italics = estimated SST</i>) ± 2 °C
			A. Z achos, Stott & Lohmann (1994)	B. Schmidt (1998, 1999)	C. Model (xaiuk) using PRISM SST dataset	D. Model (xatsb) using model SST dataset	using Zachos, Stott & Lohmann (1994)	using Zachos, Stott & Lohmann (1994) + $\delta^{18}\text{O}_{\text{sw}}$ -0.33 per mil SMOW	using Schmidt (1998, 1999)	Model (xaiuk)	Model (xatsb)			
907A <i>pach</i>	3.75	0.16	-0.25	-0.1	0.2	0.18	-2.47	-3.64	-1.94	-0.87	-0.94	2.53	3.67	
606 <i>bull</i>	0.21 - 1.05 (14)	0.34	0.44	0.8	0.61	0.62	8.9-13	7.3-11.4	10.7-14.8	9.7-13.8	9.8-13.9	19.6	21.83	21.6
603C <i>rub</i>	-0.56	0.64	0.49	1.18	0.47	0.96	17.7	16.2	20.7	17.6	19.8	23.25	25.92	26.4
603C <i>obliq</i>	0.16	0.64	0.49	1.18	0.47	0.96	14.5	13	17.5	14.4	16.6	23.25	25.92	26.4
659A* <i>sacc</i>	-0.2 to -1.27 (13)	1.5	0.84	0.7	1.21	1.93	18.3-22.9	16.8-21.5	17.7-22.3	19.9-24.5	22.9-27.7	22.72	27.52	22.5
502B <i>quad</i>	-1.56	0.17	0.84	1.14	0.11	1.54	24.2	22.7	25.4	21	27.2	27.6	27.61	27.7
925B <i>sacc</i>	-1.72	0.15	0.72	0.98	0.45	0.4	24.3	22.9	25.5	23.2	23	27.6	29.98	27.5
925C <i>sacc</i>	-1.31 to -1.82 (18)	0.15	0.72	0.98	0.45	0.4	22.6-24.8	21.1-23.3	23.7-26	21.4-23.6	21.2-23.4	27.6	29.98	27.5
516A <i>sacc</i>	0.05 - 0.79 (15)	0.16	0.63		0.3	0.32	13-16.2	11.6-14.8		11.6-14.8	11.7-14.9	21.3	22.15	23.2
516A* <i>sacc</i>	0.33 - 0.53 (4)	0.16	0.63		0.3	0.32	14.1-15	12.7-13.6		12.7-13.6	12.8-13.7	21.3	22.15	23.2
517 <i>sacc</i>	-0.13 - 0.55 (17)	0.22	0.62		0.31	0.27	14-17	12.6-15.6		12.7-15.6	12.5-15.5	21.3	22.33	22.5
704A <i>bull</i>	2.12 - 2.62 (16)	-0.28	0.16		-0.25	-0.34	-0.1 to 2.3	-1.8 to 0.7		-2.15 to 0.3	-2.6 to -0.15	5.3	7.93	8.4
704A <i>pach</i>	2.21 - 2.49 (13)	-0.28	0.16	-0.28	-0.25	-0.34	3.5-4.5	2.3-3.2	1.9-2.9	2.0-3.0	1.7-2.7	5.3	7.93	8.4

Figure 4. Calculated SSTs for nine DSDP/ODP sites/holes in the Atlantic Ocean, which yield oxygen isotope data for the interval of the Kaena Subchron. The SST estimates are derived by the equations for named species in Figure 5 (compare results with those in Fig. 6). Calcification temperatures for the various species are based on $\delta^{18}\text{O}_{\text{sw}}$ estimates using Zachos, Stott & Lohmann (1994), Schmidt (1998, 1999) and the modelled data. The $\delta^{18}\text{O}_{\text{sw}}$ value at ODP Hole 907A for ‘Schmidt’ is an absolute value at that locality derived directly from the GEOSECS website. Calculations based on the model experiments assume ice volume one third less than at present. Other calculations (columns A, B) assume ice volumes similar to present (that is, $\delta^{18}\text{O}_{\text{sw}}$ of 0.0‰ SMOW). By adding a correction factor for $\delta^{18}\text{O}_{\text{sw}}$ of -0.33‰ SMOW (for those values given in column A), accounting for an ice volume for the mid-Pliocene of two thirds present, the SSTs remain cooler than at present.

Foraminifer species	Eq. No.	Calcification temperature equation	Source reference
<i>Neogloboquadrina pachyderma</i>	1	$T (^{\circ}\text{C}) = -3.55 (d_c - d_{\text{sw}}) + 12.69$	Mulitza, Boltovskoy, Donner, Meggers, Andre & Wefer, 2003
<i>Globigerina bulloides</i>	2	$T (^{\circ}\text{C}) = -4.89 (d_c - d_{\text{sw}}) + 13.20$	Bemis, Spero, Bijma & Lea, 1998
<i>Globigerinoides ruber</i>	3	$T (^{\circ}\text{C}) = -4.44 (d_c - d_{\text{sw}}) + 14.20$	Mulitza, Boltovskoy, Donner, Meggers, Andre & Wefer, 2003
<i>Globigerinoides obliquus</i>	3	$T (^{\circ}\text{C}) = -4.44 (d_c - d_{\text{sw}}) + 14.20$	Mulitza, Boltovskoy, Donner, Meggers, Andre & Wefer, 2003
<i>Globigerinoides quadrilobatus</i> grp	4	$T (^{\circ}\text{C}) = -4.35 (d_c - d_{\text{sw}}) + 14.91$	Mulitza, Boltovskoy, Donner, Meggers, Andre & Wefer, 2003
<i>Globigerinoides sacculifer</i>	4	$T (^{\circ}\text{C}) = -4.35 (d_c - d_{\text{sw}}) + 14.91$	Mulitza, Boltovskoy, Donner, Meggers, Andre & Wefer, 2003
all species (see Fig.6)	5	$T (^{\circ}\text{C}) = 16.998 - 4.52 (d_c - d_{\text{sw}}) + 0.028 (d_c - d_{\text{sw}})^2$	Erez & Luz, 1983

Figure 5. Palaeotemperature equations used to estimate SST for the six species of planktonic foraminifera from the Atlantic sites, where δ_c (denoted as d_c in figure) is the isotopic composition of the calcite sample (relative to Vienna Pee Dee Belemnite Standard, or VPDB) and δ_{sw} (denoted as d_{sw} in the figure) is the isotopic composition of the ambient seawater (relative to Standard Mean Ocean Water, ‘SMOW’). In the calculations for palaeotemperature given in Figures 4 and 6, the $\delta^{18}\text{O}_{\text{sw}}$ SMOW values are corrected to the VPDB scale by subtracting 0.27‰ for equations 1–4, and 0.22‰ for equation 5 (see Hut, 1987; Spero *et al.* 2003). In our assessments of SST, the temperature equation used for *G. ruber* is applied to the related species *G. obliquus*, and that for *G. sacculifer* applied to *G. quadrilobatus*.

Here $\delta^{18}\text{O}_{\text{sw}}$ is the isotopic composition of the seawater ($\delta^{18}\text{O}$, SMOW) and y is the absolute latitude in the range 0 to 70°. The latitudinal correction of this equation provides a useful first approach to account for local or regional variations in $\delta^{18}\text{O}_{\text{sw}}$ (Fig. 4, column A). We have also reconstructed the present-day global distribution of $\delta^{18}\text{O}_{\text{sw}}$ using GEOSECS data and other data compiled by Schmidt (1999) and Bigg & Rohling (2000) (the full dataset of Schmidt, Bigg & Rohling 1999, Global seawater oxygen-18 database, is available at: <http://www.giss.nasa.gov/data/o18data>). In order to reconstruct a continuous surface model we employed a spatial interpolation routine based on grid averaging (Taylor *et al.* 2004). This has enabled us to make a more constrained correction for local seawater

$\delta^{18}\text{O}$ variations in our temperature calculations (Fig. 4, column B).

Both of the above methods assume that mid-Pliocene Atlantic $\delta^{18}\text{O}_{\text{sw}}$ was similar to that at present. This is a justifiable view, considering that closure of the Isthmus of Panama occurred about this time, with modern Atlantic Ocean circulation patterns established (Haug & Tiedemann, 1998; Haug *et al.* 2001). However, mid-Pliocene ice-volumes may have been up to a third less than at present (Webb *et al.* 1984; Haywood & Valdes, 2004). The different volume of the Antarctic Ice Sheet is already factored into those calculations of $\delta^{18}\text{O}_{\text{sw}}$ derived by the modelling experiments (Fig. 4, columns C, D). Recalculating values for column A in Figure 4, with a correction factor for $\delta^{18}\text{O}_{\text{sw}}$

ODP/ DSDP Site and foram. species	Foraminifer calcite - $\delta^{18}\text{O}$ [VPDB], for Kaena subchron interval (3.12Ma to 3.05Ma)	Local delta $^{18}\text{O}_{\text{sw}}$ [SMOW]		Mean SST		PRISM2 SST - mean annual (<i>italics = estimated SST</i>) ± 2 °C
		Present estimated (model Xajpa)	Model (xatsb) using model SST dataset	Model estimated (xatsb)	Present mean annual temper- ature	
907A <i>pach</i>	3.75	0.16	0.18	0.27	2.53	
606 <i>bull</i>	0.21 - 1.05 (14)	0.34	0.62	17.9 max	19.6	21.6
603C <i>rub</i>	-0.56	0.64	0.96	22.9	23.25	26.4
603C <i>obliq</i>	0.16	0.64	0.96	19.6	23.25	26.4
659A* <i>sacc</i>	-0.2 to -1.27 (13)	1.5	1.93	25.4-30.7	22.72	22.5
502B <i>quad</i>	-1.56	0.17	1.54	30.3	27.6	27.7
925B <i>sacc</i>	-1.72	0.15	0.4	25.7	27.6	27.5
925C <i>sacc</i>	-1.31 to -1.82 (18)	0.15	0.4	23.8 max	27.6	27.5
516A <i>sacc</i>	0.05 - 0.79 (15)	0.16	0.32	17.2 max	21.3	23.2
516A* <i>sacc</i>	0.33 - 0.53 (4)	0.16	0.32	15.7max	21.3	23.2
517 <i>sacc</i>	-0.13 - 0.55 (17)	0.22	0.27	17.8 max	21.3	22.5
704A <i>bull</i>	2.12 - 2.62 (16)	-0.28	-0.34	5.1 max	5.3	8.4
704A <i>pach</i>	2.21 - 2.49 (13)	-0.28	-0.34	4.7 max	5.3	8.4

Figure 6. Calculated SSTs for nine DSDP/ODP sites/holes in the Atlantic Ocean, which yield oxygen isotope data for the interval of the Kaena Subchron. The estimates are based on equation (5), which may overestimate SSTs (see Mulitza *et al.* 2003). Calcification temperatures for the foraminifera are based on $\delta^{18}\text{O}_{\text{sw}}$ reconstructions from the coupled ocean atmosphere model (Fig. 4).

of -0.33‰ SMOW does not affect our conclusions. Lear, Elderfield & Wilson (2000) suggested $\delta^{18}\text{O}_{\text{sw}}$ of about -0.54‰ SMOW for the mid-Pliocene, which also concurs with an ice sheet somewhat smaller than at present. Substituting this figure in the equations used in Figure 5 also produces SST estimates cooler than at present for the data of Figures 4 and 6 (calculations not shown).

The interpretation of mid-Pliocene $\delta^{18}\text{O}_{\text{sw}}$ based on climate modelling studies uses the HadCM3 General Circulation Model. Model calculated values for the $\delta^{18}\text{O}_{\text{sw}}$ are an attempt to capture longitudinal and latitudinal change in $\delta^{18}\text{O}_{\text{sw}}$ as a function of climate, and are based upon precipitation minus evaporation (P – E) estimates derived from the climate model. Present-day observed $\delta^{18}\text{O}_{\text{sw}}$ is calibrated against observed P – E. The resulting formula (see below) is used to predict $\delta^{18}\text{O}_{\text{sw}}$ gradients for the mid-Pliocene.

$$\delta^{18}\text{O}_{\text{sw}} = 0.1725 - 0.008(P - E) \quad (7)$$

$\delta^{18}\text{O}_{\text{sw}}$ for the mid-Pliocene is estimated from two model experiments, one calibrated with PRISM SSTs (model xaiuk), the other using SSTs calculated by the model itself (model xatsb, coupled ocean atmosphere run); for technical information regarding HadCM3, its set-up and experimental design for the mid-Pliocene, see Haywood & Valdes (2004) or Haywood *et al.* (2005). The temperature values that we calculate are clearly subject to temperature/climate variation within

the 70 000 years of the Kaena Subchron. Nevertheless, the data yield largely uniform trends, even from those sequences where isotopic data are available from several horizons (Fig. 7a,b).

3. Oxygen isotope SST estimates compared with those of PRISM and a fully coupled ocean–atmosphere GCM for the mid-Pliocene

The ‘PRISM Time Slab’ is climatically distinct, but substantial climatic variability occurs within it. Because of this, PRISM developed the ‘peak averaging’ method (Dowsett & Poore, 1991; Dowsett *et al.* 1994) to estimate mean interglacial conditions within the interval and minimize problems associated with long-distance absolute correlations. The Kaena Subchron of the Gauss Normal Polarity Chron represents a sub-interval within the ‘PRISM Time Slab’ that was unaffected by major oxygen isotope excursions (G20, KM2, M2 and MG2) that equate to more extensive polar ice sheets (see Shackleton *et al.* 1995), and cooler climate (Haywood, Valdes & Sellwood, 2002). Thus, analysis of the isotopic signature of the planktonic foraminifera at the sites studied here should be expected to yield results with similar or warmer SST conditions than at present, given that the PRISM interval equates to an overall warmer climate. Five of the sites have also yielded fossil assemblage data to PRISM (Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999). However,

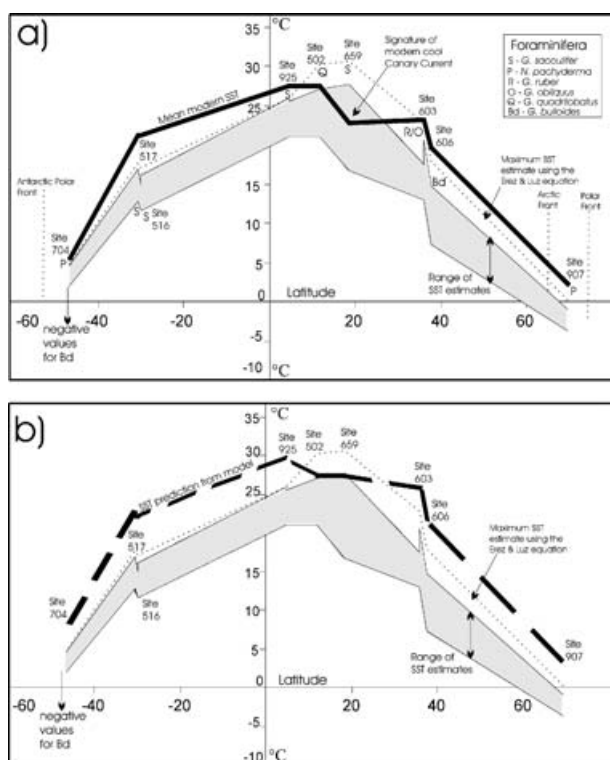


Figure 7. Reconstruction of SST from data summarized in Figures 4 and 6. The lowest and highest SST estimate at each site are plotted from Figure 4 (grey area) and the warmest SST estimate using the Erez & Luz (1983) equation is indicated by the thin dotted line. In (a) the bold line represents modern SST based on data from Smith & Reynolds (1998) and Reynolds & Smith (1995). In (b) the thick dotted line is the SST predicted from the coupled ocean atmosphere model. Note that at ODP Site 659 the total dataset probably includes horizons older and younger than the Kaena Subchron. The relative position of the modern Polar, Arctic and Antarctic Polar fronts are marked in relation to ODP sites 704 and 907.

in contrast to the PRISM fossil dataset and the SSTs predicted by the GCM, most of the estimated SSTs using the planktonic foraminifer oxygen isotope data suggest cooler SSTs, and this is particularly the case using the $\delta^{18}\text{O}_{\text{sw}}$ estimates derived from the climate model calibrated with PRISM2 SSTs (Dowsett *et al.* 1999) as a prescribed boundary condition (Fig. 4).

Two sites in the North Atlantic north of 30° latitude (DSDP 603C, 606) that give warmer than present SSTs for February and August according to PRISM (based on planktonic foraminifer assemblages) and the GCM, both yield isotopic data for the Kaena Subchron that suggest SST several degrees cooler than at present (Figs 4,7a). Cooler SST is estimated at DSDP Hole 603C from the $\delta^{18}\text{O}$ of *Globigerinoides ruber* and *Globigerinoides obliquus* calcite. At DSDP Site 606, cooler SST is consistent from 11 analyses of *Globigerina bulloides* through this interval (Fig. 4). Similarly, at South Atlantic DSDP Hole 516A and ODP Site 704, PRISM and the GCM predict warmer SST, whilst the isotopic data from *Globigerinoides sacculifer*, *Ne-*

globoquadrina pachyderma and *Globigerina bulloides* in the Kaena Subchron estimate cooler temperatures, through a range of analyses in this interval, with temperatures sometimes more than 5°C cooler than present SST (Fig. 7a,b). Cooler SSTs in the Atlantic south of 30° latitude are also indicated by oxygen isotope data from DSDP Site 517 (Fig. 7a, b).

At ODP Hole 502B, in the tropics, PRISM and the GCM estimate SST very similar to modern ($=27.6^\circ\text{C}$; see Fig. 4). The SST estimates at this site (from the $\delta^{18}\text{O}$ data) range from cooler (21°C) to warmer (30.3°C ; Figs 4, 6), though the mean temperature estimate (25.7°C) is cooler, and the maximum temperature value here is probably an overestimate due to the use of the Erez & Luz (1983) equation (see Mulitza *et al.* 2003). Cooler SSTs in the tropics are also estimated for ODP Site 925 (Fig. 7a,b). At ODP Hole 659A, off the coast of West Africa (modern SST at this site is 22.72°C), temperature estimates are more equivocal, with $\delta^{18}\text{O}_{\text{sw}}$ estimates from the coupled ocean atmosphere and PRISM2 calibrated Pliocene climate models producing warmer SST (maximum values are 24.5°C and 27.7°C ; Fig. 4), and the other methods for assessing $\delta^{18}\text{O}_{\text{sw}}$ providing estimates of temperature very similar to present (maximum values in the range 21.5 – 22.9°C ; Fig. 7a,b). Data from alkenones at ODP Site 958, also off the northwest coast of Africa, give SST of 23.1°C at 3.07 Ma (Herbert & Schuffert, 1998). This is warmer than estimated SSTs for the interval post-2.5 Ma at this site, but slightly cooler than the average SST (25.3°C) for the interval 6.5 to 2.2 Ma. PRISM estimated little or no change between mid-Pliocene SST and present SST at low latitudes (Dowsett *et al.* 1999), though the GCM supported by data from alkenones at Pacific ODP sites 847, 1014 and 1237 suggests warmer sea temperatures in the tropics (see also Haywood & Valdes, 2004; Haywood *et al.* 2005).

4. Why do the oxygen isotope data suggest a cooler ocean surface?

The temperature estimates from the foraminifer tests give a latitudinal variation similar to that of modern SSTs. However, estimates are generally several degrees cooler than at present and much cooler than SST estimates for the mid-Pliocene from PRISM and the GCM (Fig. 7a,b). The foraminifer calcite is, at least in part, reflecting original Pliocene latitudinal SST variation. The cooler SST signals from the oxygen isotope data can be interpreted either as a flaw in the assessment of the original fossil/isotope data, as a real signal, as a taphonomic effect, or as an ecological or physiological effect during the life of the organisms. In the first category are problems associated with the interpretation of fossil assemblages, which may be causing mean SST overestimates for the interval 3.29 to 2.97 Ma, or problems of $\delta^{18}\text{O}_{\text{sw}}$ estimation, or poor stratigraphy. In the second category, if we accept that

the signal from the isotopes is real, these data contradict some of the conclusions presented by PRISM and the prediction of mid-Pliocene SSTs generated by the GCM. Also, in the third and fourth categories, the isotope signal of the foraminifer calcite may have been reset by taphonomic processes (diagenesis or dissolution), or by processes during the life of the organisms.

4.a. SST estimates from PRISM and the GCM

4.a.1. PRISM estimates

Faunal assemblage estimation techniques for SST assume that the composition of planktonic foraminifer assemblages is related to SST (Andersson, 1997). The distribution of surface-dwelling planktonic foraminifera in the world's oceans is linked to a range of optimum SSTs (Bé & Hutson, 1977), but nutrient supply, water salinity and other environmental factors are important (Hemleben, Spindler & Anderson, 1989). The most significant problem associated with pre-Quaternary SST estimation involves differences between modern and fossil assemblages. To overcome this, the PRISM Group assumed that species belonging to the same evolutionary lineage have the same environmental preferences (Dowsett & Poore, 1991; Dowsett, 1991). This, however, removes the possibility that new species within a lineage evolved as the result of changing surface ocean properties (Andersson, 1997). The problem of 'taxonomic uniformitarianism' can be partly overcome by comparing one fossil dataset to another. The PRISM Group undertook such a procedure for the North Atlantic. Foraminifera, ostracods and microflora all gave similar results in the magnitude and direction of Pliocene climate change. For example, during the mid-Pliocene, areas of Iceland now covered by tundra vegetation were covered by deciduous forest, suggesting temperatures 3° to 5°C warmer than today (Willard, 1994). Ostracods and foraminifera also indicate a warmer North Atlantic during the warm intervals of the mid-Pliocene (Cronin, 1991a,b; Dowsett & Poore, 1991; Dowsett *et al.* 1992). Thus, different organisms show a common climatic signal, increasing confidence in the original methods used in reconstructing SSTs for the mid-Pliocene.

Nevertheless, at ODP Site 646B in the Labrador Sea, Dowsett & Poore (1991, p. 198) noted a discrepancy between SST estimates from planktonic foraminifera, and markedly warmer estimates given by the dinoflagellate assemblage of a single sample (up to 15°C warmer for summer). They also noted (Dowsett & Poore, 1991, p. 198) that the planktonic foraminifer assemblages at DSDP Site 606 may not provide accurate assessments of SST. In reality then, there is no way to address completely the problems presented by taxonomic uniformitarianism in SST reconstruction, though the huge dataset evaluated by PRISM suggests

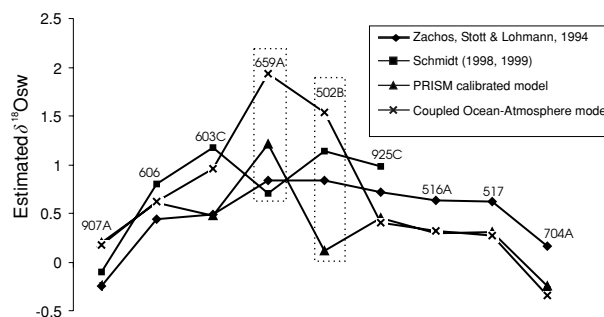


Figure 8. Estimated $\delta^{18}\text{O}_{\text{sw}}$ for the Kaena Subchron based on the methods summarized in the text. The data for this graph are sourced from Figure 4, columns A–D. At two sites the variation in estimated $\delta^{18}\text{O}_{\text{sw}}$ exceeds 1.0‰ (marked by boxes), which has a significant affect on the range of estimated SSTs at sites 502 and 659.

this may be a minor factor in the offset between temperature estimates from fossil assemblages, and those from oxygen isotopes. PRISM placed confidence values of $\pm 2^\circ\text{C}$ on their SST estimates (Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999). At the sites we evaluate here, this means that the minimum mean annual SST estimates of PRISM are at least as warm as at present (Fig. 4).

4.a.2. GCM estimates

As already noted above, the coupled ocean–atmosphere GCM, like PRISM, also estimates warmer conditions than at present for the mid-Pliocene (Fig. 7b), though it predicts warmer temperatures both for the tropics and higher latitudes (see Haywood *et al.* 2005 for a discussion of mid-Pliocene climate). At all of the sites where we examine the SST signature of the oxygen isotopes, bar ODP Site 659, the model predicts SSTs several degrees warmer (Figs 4, 7b). At ODP Site 659, maximum estimates from the oxygen isotope data (27.7°C) are very similar to the GCM prediction at this site (27.52°C), though minimum SST estimates at this site are as low as 16.8°C (Fig. 4).

4.b. Accuracy of estimating $\delta^{18}\text{O}_{\text{sw}}$

The variation in surface seawater isotopic composition ($\delta^{18}\text{O}_{\text{sw}}$; Fig. 8) produced by the methods documented above (Section 2.b) inevitably leads to differences in the calcification temperatures calculated for the foraminifer tests. Difficulties estimating $\delta^{18}\text{O}_{\text{sw}}$ have been cited as a reason for discrepancies between SST estimates from fossil assemblages and those from oxygen isotopes for the Last Glacial Maximum at 18 ka (Wolff *et al.* 1998). For example, at temperatures between 24 and 28°C , a change in $\delta^{18}\text{O}$ of 0.22‰ SMOW is equivalent to a temperature difference of 1°C (Wolff *et al.* 1998). At most mid-Pliocene sites, the variation between individual estimates of $\delta^{18}\text{O}_{\text{sw}}$

(Figs 4, 8) is less than 0.6‰ SMOW, resulting in SST calculations differing by less than 3 °C. However, the total range of temperature difference for all estimations at each site usually lies between 5 and 10 °C (Figs 4, 7a,b), partly reflecting $\delta^{18}\text{O}_{\text{sw}}$ values that sometimes vary overall by more than 1.0‰ SMOW, and suggesting that one or more of these $\delta^{18}\text{O}_{\text{sw}}$ estimates may be unrepresentative (Fig. 8; e.g. at DSDP Hole 502B and ODP Hole 659A). Although this may be a factor causing some of the cooler temperature estimates, the overall trend of SST estimates for most sites (except ODP Site 659) is unidirectional, and the latitudinal pattern is the same for all reconstructions (Figs 4, 6, 7a,b). In the mid-Pliocene dataset it is the isotopic composition of the foraminifer calcite, rather than the estimated $\delta^{18}\text{O}_{\text{sw}}$ that is the most influential component influencing the SST estimates. Hence, this methodology appears to produce a trend of latitudinal temperature variation that is robust, though the interpretation of absolute values is much less certain.

4.c. Chronology

Problems of correlation for the interval of the Kaena Subchron could lead to horizons of different age being compared in the dataset of Figures 3 and 4, producing errors in the comparative dataset for SST estimations for this time-slice. For example, if correlation were slightly offset to horizons younger or older than the Kaena Subchron, it is possible that levels within the KM2 and G20 isotope stages could be evaluated. These are associated with intervals when polar ice volume was probably greater than at present (Shackleton *et al.* 1995), and global climate cooler (Haywood, Valdes & Sellwood, 2000). Correlation would be a more serious problem if we were examining the isotope data from the whole of the PRISM 'Time Slab', where climatic variation was much greater than in the Kaena Subchron (see Dowsett *et al.* 1999).

An additional factor for the stratigraphy is disruption of core material during its journey from the seabed to the surface, which may have affected its continuity. Core recovery technology certainly improved over the period of the early 1980s to late 1990s, the time interval during which the boreholes analysed here were collected (see Fig. 3a,b). Some authors comment on the suitability of the cores for isotopic analysis because of minimal disturbance during coring (e.g. Hodell & Ciesielski, 1991, p. 409).

The chronology of the sites documented here is based on published accounts of the magnetochronology, astrochronology and biochronology (Fig. 1). For each of the sites we indicate the core interval from which the isotope data have been analysed (Fig. 3a), and which we believe represents the interval of the Kaena Subchron. Isotope data from sites where the chronology is less well constrained for this interval (e.g. DSDP Site 398)

have been deliberately excluded. Thus, at DSDP Site 606 there is a complete sequence of palaeomagnetic reversals through the past six million years (Clement & Robinson, 1987). This places the interval of the Kaena Subchron between depths 94.28 m and 100.25 m and is supported by the LO (last occurrence) of *D. altispira* at 99.55 m (see also Weaver & Clement, 1987, p. 819). Magnetochronology also underpins correlation at holes 502B, 603C, 704A and 907A (see Kent & Sparioso, 1982; Shipboard Scientific Party, 1987; Canninga, Zijderveld & van Hinte, 1987; Hailwood & Clement, 1991; Shipboard Scientific Party, 1995a). At DSDP Hole 603C, Core 15,CC (Fig. 3a,b) is within foraminifer zone PL4 according to Ma'alouleh & Moullade (1987). At DSDP Hole 502B the LO of *D. altispira* at 72.89 m and LO of *Sphaeroidinellopsis* at 78.8 m are additional indices constraining the interval of the Kaena Subchron (Keigwin, 1987). At ODP Hole 659A, chronology is based on the LO of *D. altispira* at depths 83.8–84.8 mbsf and of *Sphaeroidinellopsis* at 87.5–90.5 mbsf (Shipboard Scientific Party, 1988). However, these biochronological markers give ages that are slightly different from those recorded by Tiedemann (1991; see supporting datasets for oxygen isotopes at <http://www.pangaea.de/>), hence we have included a range of data at this site that might encompass a slightly longer time interval. There is no magnetochronology at ODP Site 925 because of overprint problems (Shipboard Scientific Party, 1995b, p. 80). However, an astrochronological age of 3.07 Ma is specified at depth 88.65 mbsf in Hole 925C (Chaisson & Ravelo, 1997 and references therein), and this lies close to the LO of *D. altispira* (3 Ma \pm 0.28) at depth 90.09 to 90.66 mbsf (Shipboard Scientific Party, 1995b, p. 76). Depths given by Franz (1999) for Hole 925C are composite. Foraminifer index species specify the interval of the Kaena Subchron at DSDP sites 516A and 517. Dowsett (1989) has demonstrated that key biochronological indices, including the LO of *D. altispira* and *Sphaeroidinellopsis*, can be diachronous over wide areas of the oceans, and may vary by as much as 95 000 years (see also the dataset of Wolf-Welling, T.C.W., Brenner, W., Mienert, J. & Thiede, J. 1997. SYNATLAN-database biochronostratigraphy of Atlantic DSDP/ODP drill sites, available via the Leibniz-Institut für Meereswissenschaften at the University of Kiel (IFM-GEOMAR) at <http://www.geomar.de/~twolf/ListADMModels.html>). Nevertheless, at DSDP sites 516A and 517, the LO of *D. altispira* can be considered as 'essentially synchronous' (Dowsett, 1989, pp. 8, 23).

4.d. Physiological or ecological effects

The $\delta^{18}\text{O}$ values from planktonic foraminifer tests provide a record of their calcification temperatures, but to relate these values to SST requires a detailed understanding of the ecology and physiology of

individual species. Several studies have demonstrated that effects such as photosynthesis of symbiotic algae (Spero & Lea, 1993), shell calcification and ontogeny (Spero & Lea, 1996) and carbonate chemistry (Spero *et al.* 1997) may influence the degree to which foraminifer calcite produces equilibrium with seawater. In addition, deviation of inferred temperature from the ambient surface water value at the time of foraminifer test calcification may occur because of so-called physiological ‘vital effects’ in some species (see Bemis *et al.* 1998).

The sites used to assess Pliocene Atlantic Ocean SSTs in this study yield calcification temperatures for six species of surface dwelling or near surface dwelling planktonic foraminifera. The ecology and physiology of most of these species is well constrained and most of them are extant (e.g. Spero & Lea, 1996; Mulitza *et al.* 2003). Indeed, the temperature equations developed by Mulitza *et al.* (2003) by analysis of plankton tow material of *G. bulloides*, *G. sacculifer* and other species (for supporting datasets see the Pangaea Database, <http://www.pangaea.de/home/smulitza/>) provide temperature estimates within 1°C of the ambient surface water temperature.

There are fewer problems associated with the palaeoecological interpretation of Pliocene foraminifera than there are, for example, with Late Cretaceous or Early Tertiary forms, as many Pliocene species are extant. Nevertheless, it is possible that environmental factors may have biased the results towards cooler SST estimates. For example, although typically inhabiting the mixed-layer, during their life cycle, *G. ruber*, *G. sacculifer*, *G. bulloides* and *N. pachyderma* produce gametogenic calcite, formed at greater depths (Erez & Luz, 1983; Niebler, Hubberton & Gersonde, 1999), so that calcification temperatures for these species may be averaged towards cooler values (see also Schmidt & Mulitza, 2002). This is probably an important factor contributing to cooler temperatures in the Kaena Subchron dataset. Although specimens of *G. sacculifer* without a gametogenic ‘sac-like’ structure were analysed at DSDP sites 516A and 517 (see Leonard, Williams & Thunell, 1983, p. 897) and ODP Site 925, Bé (1980) notes the presence of gametogenic calcite in specimens without a sac-like structure. Such specimens might be difficult to discern without detailed scanning electron microscopy. Analysis of *G. sacculifer* from modern core top sediments, mostly from the Atlantic Ocean (Fig. 9), indicate that processes influencing a ‘cooler than ocean surface’ temperature signal from the foraminifer calcite do indeed occur at an early (pre-fossil) stage, supporting the argument that this involves calcite formed below the ocean mixed-layer (and below the level from which plankton tow material has been analysed for its temperature signature) during the life cycle of the foraminifer. Indeed, many of the specimens of *G. sacculifer* that we have examined from ODP sites 659 and 925 have a secondary calcite

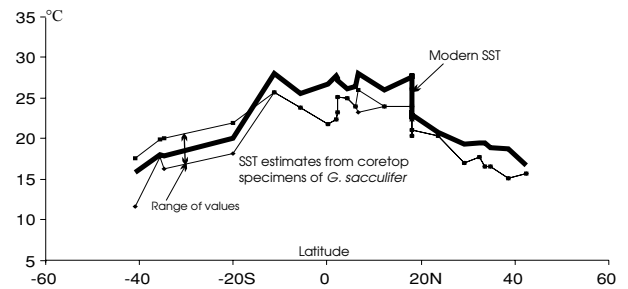


Figure 9. SST estimates from 25 sites with core top material of *G. sacculifer* (dataset of Stefan Mulitza, University of Bremen, in the Pangaea database: <http://www.pangaea.de/home/smulitza/>). Estimates are typically 0–3°C cooler than actual SSTs, though the discrepancy is greater in tropical regions. SST estimates use the equation of Zachos, Stott & Lohmann (1994) for the calculation of $\delta^{18}\text{O}_{\text{sw}}$. The data indicate that processes causing cooler estimates of SST take place early (pre-fossil), and probably include calcite formed near the base of, or below the ocean mixed-layer during the life of the foraminifera, mixing of assemblages from cool and warm climatic intervals by bioturbation, and selective dissolution of foraminifer tests (see Mulitza *et al.* 2004).

overgrowth that is probably gametogenic (Fig. 10a–c, e, g). Some of the temperature discrepancy may also be related to the depth of the chlorophyll maximum zone (Waelbroeck *et al.* 2004). During periods of stratification of the upper water column, temperatures at the chlorophyll maximum may differ by several degrees from surface temperatures (Fairbanks & Wiebe, 1980). The temperature difference estimated by the core top material, typically 0–3°C cooler than the ocean surface, is less than in the mid-Pliocene dataset (mean temperature difference for *G. sacculifer* is typically 4–5°C cooler than at present, though minimum SST estimates can be much cooler; see Fig. 4), so that these effects do not fully explain the temperature discrepancy in the fossil material. However, in equatorial regions, modern core top material sometimes yields SST estimates 5°C cooler than actual (see Fig. 9), so that calcite formed in the foraminifer shells at depths near the base of, or below the mixed-layer, might have a significant influence on the temperature signal of the foraminifer tests at some sites.

Although it typically occurs within the mixed layer, *N. pachyderma* may provide only a general indication of sea temperature through a relatively thick part of the water column (Bauch, Carstens & Wefer, 1997). Whilst the signal from *N. pachyderma* is useful for identifying water mass changes as a result of climatic shifts, its use as an indicator of SST from fossil material may be more limited. In the dataset analysed here, *N. pachyderma* yields SST estimates somewhat cooler than at present for both the Arctic Sea (ODP site 907A, estimates typically 3–6°C cooler than at present, Fig. 4) and southern Atlantic (ODP site 704, typically 1–3°C cooler than at present, Fig. 4). At the latter site this cool signal is

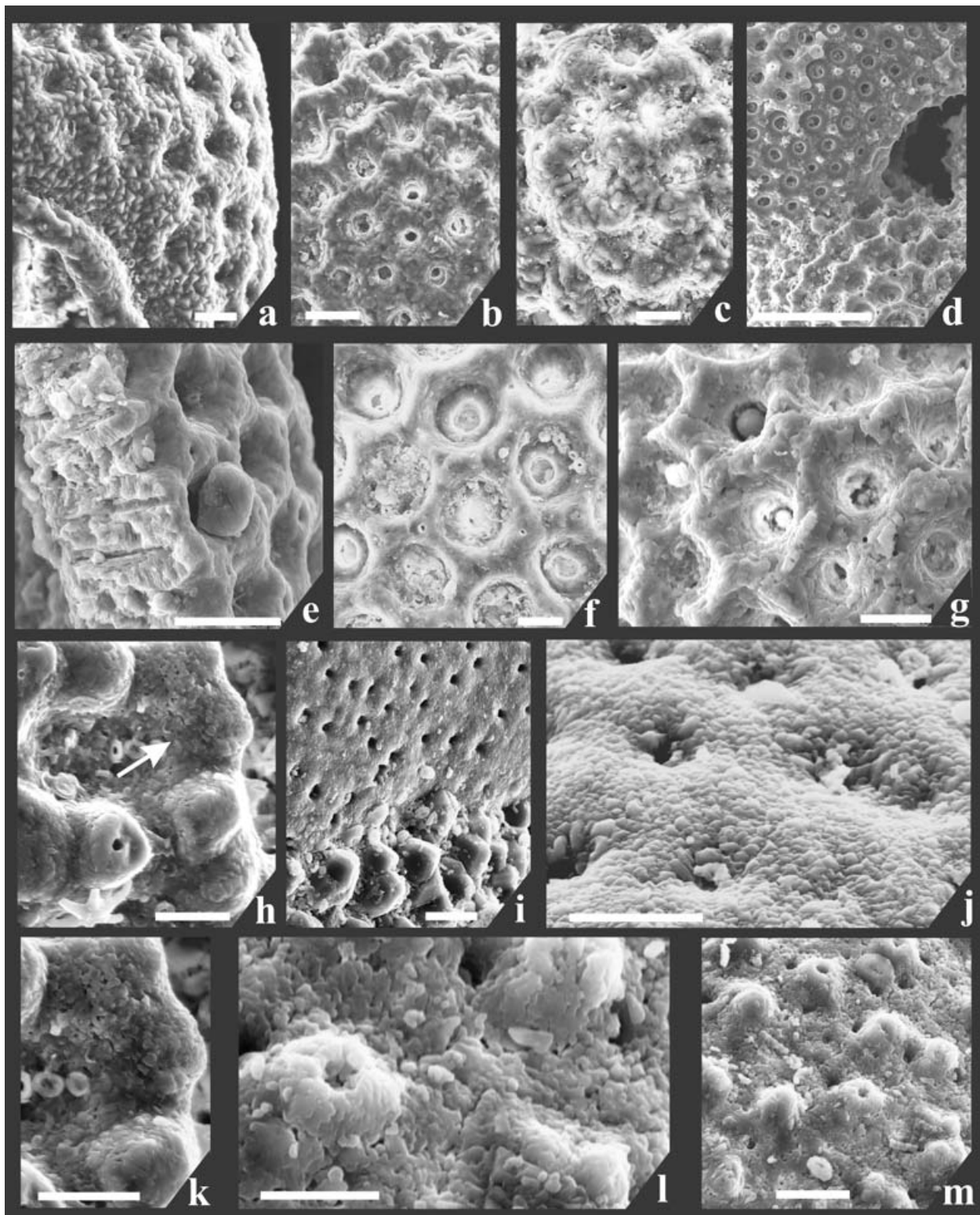


Figure 10. Scanning electron micrographs of mid-Pliocene planktonic foraminifera from ODP holes 659A (core 10H-4, 140–144 cm; c, f, g), 704A (core 19X-6, 20–24 cm; i, j, l, m) and 925B, 925C (cores 10H-6, 63–67 cm and 10H-6, 21–25 cm respectively; a, b, d, e, h, k) (see Fig. 1 for localities). The original sediment source (calcareous/nannofossil oozes) for the foraminifera was dissociated in de-ionized water without agitation, normally for a period of 24 hours. No Calgon was introduced, hence the surfaces of some of the foraminifera still have sediment residue sticking to them (including coccolithophores). Sediment residues were sieved, and oven dried at a temperature not exceeding 50 °C. (a–h, k) *Globigerinoides sacculifer*; (i, j) *Neogloboquadrina pachyderma*; (l, m) *Globigerina bulloides*. (a–c) Calcite veneer overgrowing the test of specimens with sac-like structures (cf. Bè, 1980, pls 7, 8). (d) Partial dissolution of the test wall. (e) Cross-section through test wall of broken specimen. The irregular surface of the test indicates a secondary calcite veneer, but the original test wall does not show recrystallization. (f) Outer surface of specimen showing closure of some pore pits by secondary calcite. (g) Secondary calcite veneer on test surface around pore pits. This specimen is from the same sample as

Table 1. Sea surface temperatures calculated from the isotopic signature of foraminifera derived from the same horizons as those specimens in Figure 10 (from published $\delta^{18}\text{O}$ data; see Figs 3a,b, 4)

Leg/Site/Hole	Core sampled	Depth (mbsf)	Foraminifer	Lithology	$\delta^{18}\text{O}$ (VPDB)	SST estimate	Present SST
108-659A	10H-4, 142–144 cm	89.68	<i>sacculifer</i>	nannofossil ooze	-0.74	20.6	22.72
114-704A	19X-6, 22–24 cm	176.23	<i>pachyderma</i>	siliceous/calcareous ooze	2.44	3.6	5.3
114-704A	19X-6, 22–24 cm	176.23	<i>bulloides</i>	siliceous/calcareous ooze	2.4	0.9	5.3
154-925B	10H-6, 63–65 cm	88.65	<i>sacculifer</i>	nannofossil ooze	-1.72	24.9	27.6
154-925C	10H-6, 22–24 cm	91.73	<i>sacculifer</i>	nannofossil ooze	-1.82	25.3	27.6

SST estimates use the equation of Zachos, Stott & Lohmann to derive $\delta^{18}\text{Osw}$. Offsets from present are in the order of 2 to 3 °C cooler.

consistent for 14 horizons through the interval of the Kaena Subchron with $\delta^{18}\text{O}$ data, and is supported by similarly cool SST estimates from *G. bulloides* (Fig. 4). Specimens of *N. pachyderma* at ODP Site 704 show development of a secondary calcified crust, formed during ontogenesis (Fig. 10i; see Henrich, 1989). This crystalline morphotype is adapted for waters cooler than 8 °C (Reynolds & Thunell, 1986).

G. bulloides is a spring bloom species associated with enhanced upwelling and productivity, reaching its highest abundance at the depth of the chlorophyll maximum zone (Ganssen & Kroon, 2000; King & Howard, 2003). In the northern hemisphere it is a species typical of the spring bloom and records SSTs for February and March between 30° and 40° N (Ganssen & Kroon, 2000; Elderfield & Ganssen, 2000). PRISM2 estimated February SST at ODP Site 606 of 17.58 °C (Dowsett *et al.* 1999). Through 14 analyses at this site the oxygen isotope data from *G. bulloides* record SSTs typically more than 5 °C cooler than at present for the Kaena Subchron (Fig. 4), with SST estimates sometimes as low as 8.9 °C. Thus, oxygen isotope data from DSDP Site 606 (37.34° N) may have been biased both by spring temperatures, and by calcite formed at levels deeper in the water column.

4.e. Taphonomic effects

Masking of the primary oceanographic signal of planktonic foraminifer tests may occur because of diagenetic overprinting. Both calcitic overgrowths and dissolution of the foraminiferal tests during early burial tend to bias results to isotopically heavier values and 'cooler' temperatures (Savin & Douglas, 1973; Killingley, 1983; Isern, McKenzie & Feary, 1996; Mulitza *et al.* 2004). Pearson *et al.* (2001)

demonstrate that the micro-granular construction of the planktonic foraminifer test is susceptible to diagenetic recrystallization. They suggest that early diagenetic alteration in sea bottom pore waters with higher $\delta^{18}\text{O}$, taking the form of fine-scale recrystallization, may be more pervasive than originally recognized, adding a further complication in palaeotemperature reconstruction. In contrast, deeper burial (probably at depths greater than 300 m), with recrystallization in pore waters that have lower $\delta^{18}\text{O}$, will result in the opposite effect, with 'warmer' temperature estimates (Schrag, DePaolo & Richter, 1995).

We have noted the preservation quality of the foraminifer tests from which the Atlantic isotopic data are derived, reported in the original source papers for our data (Fig. 3b). In most cases, material was assessed to be well preserved, or even excellent (e.g. Ganssen, 1987, p. 997; Leonard, Williams & Thunell, 1983, p. 895; Ehrmann & Keigwin, 1987, p. 921; Dowsett, 1989, p. 8; Hodell & Cieselski, 1991, p. 410; Chaisson & Pearson, 1997, p. 11), but, for example, dissolution of foraminifer tests at DSDP Hole 603C (Dowsett & Poore, 1991, p. 198) may have contributed to cooler SST estimates there. Mulitza *et al.* (2004, fig. 5) indicate that dissolution, or the effects of bioturbation bringing older (glacial episode) material to the surface, occur relatively rapidly after the tests of planktonic foraminifera reach the sea bottom, resulting in material with higher $\delta^{18}\text{O}$ values. The $\delta^{18}\text{O}$ values of planktonic foraminifera carbonate from core top sediments sometimes yield good estimates of modern SST, but in other cases, the SST estimates differ by several degrees, and can be much cooler (see Mulitza *et al.* 2003 for further discussion; see also the dataset available at: <http://www.pangaea.de/home/smulitza/>). In the small mid-Pliocene dataset analysed here, there

(f), indicating the range of preservation that can occur at a single site. (h, k) Fine-scale recrystallization of test surface around pore pits (arrowed), and close-up of detail. (i, j) *Neogloboquadrina pachyderma* (sin.). (i) Detail of the secondary calcite crust formed over all but the youngest chamber of the test. For comparison, see Henrich (1989, plate 2, fig. 9). This crust forms during the life of the foraminifer. (j) Surface of youngest chamber with calcite crystals coarsening into the margins of the pores. (l, m) Details of the surface of a specimen with well-preserved spine bases, but showing fine-scale recrystallization of the test surface. Contrast with plankton tow specimens figured by Cifelli (1982, pl. 9; see also Dittert & Henrich, 2003). Scale bar: (a, c, f–k, m) = 10 μm ; (b, e) = 20 μm ; (d) = 70 μm ; (l) = 5 μm . All specimens are deposited in the collections of the British Antarctic Survey, Cambridge, UK. Sea surface temperature estimates for material from these horizons are given in Table 1.

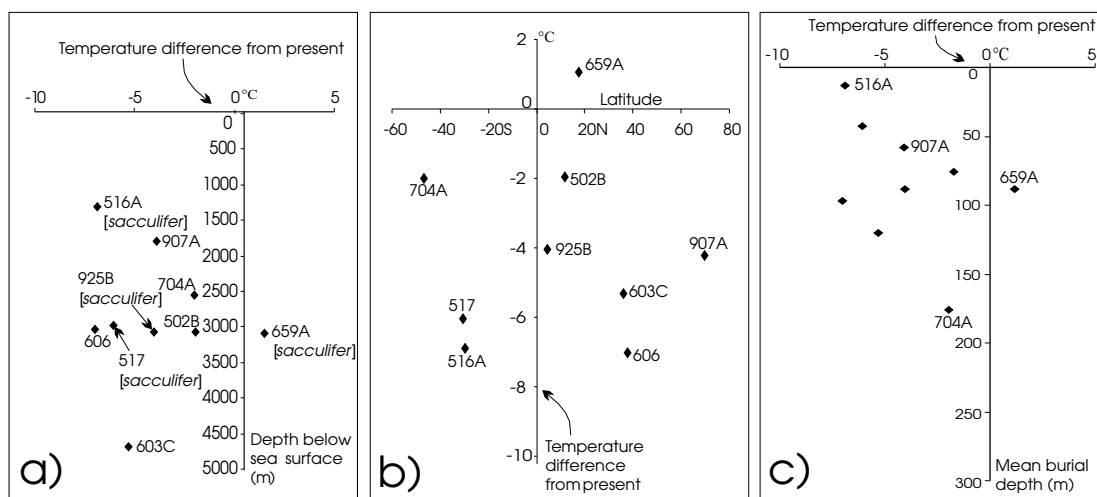


Figure 11. Average temperature difference from present, given by isotopic data from planktonic foraminifera of the Kaena Subchron at the chosen sites of Figure 3a,b, plotted against: (a) water depth in the Atlantic (given as depths below sea level), (b) latitude and (c) mean burial depth. For DSDP Hole 603C the mean temperature is the average of values for *G. ruber* and *G. obliquus*. For ODP Hole 704A, the mean temperature is based on *N. pachyderma*. There is no simple correlation between greater water depth and cooler SST estimates, as might be expected if dissolution was the key factor shifting the temperature signal of the foraminifer calcite to cooler estimates (see Mulitza *et al.* 2004), though dissolution susceptibility varies between the different species, with *N. pachyderma* least susceptible and *G. bulloides* very unstable (see Berger, 1971). In (c), there is a suggestion (though this is not statistically significant) that greater burial depth yields SST estimates less negative from present, suggesting that possible later burial diagenetic processes have reset the isotopic signature of the calcite.

is no simple correlation between increased dissolution (causing higher $\delta^{18}\text{O}$ values for the foraminifer calcite, and shifting temperature estimates toward cooler SST estimates), and greater modern water depth (Fig. 11a). This is also suggested by the adjacent DSDP sites 516 (1313 m water depth) and 517 (2963 m water depth), which provide a similar range of SST estimates from the dissolution susceptible *G. sacculifer* (Fig. 7a,b). Bioturbation, mixing assemblages from climatically cooler and warmer intervals, is also less of an issue in the time-averaged assemblages from the Kaena Subchron, particularly at those sites with isotopic data from several horizons. Nevertheless, data from modern core top planktonic foraminifera (Fig. 9) suggest that dissolution (and mixing of assemblages by bioturbation) may play a role in cooler SST estimates from the foraminifer calcite.

Isotopic evidence from benthic foraminifera suggests less extensive polar ice sheets during the Kaena Subchron interval (Shackleton *et al.* 1995), which together with a wide range of fossil data, probably indicate a warmer climate. Thus, the dominantly cool temperature signature of the planktonic foraminifera compared to present SSTs and PRISM reconstructed SSTs may also identify an early diagenetic calcite phase, with higher $\delta^{18}\text{O}$, causing the cool temperature signature across a range of latitudes and for several different species. Pearson *et al.* (2001) note a similar discrepancy between the Greenhouse climate of the Late Cretaceous and Early Tertiary, and SST estimates from planktonic foraminifera in the palaeo-tropics that suggest surface waters of only 15°C to 23°C at that

time, though Cretaceous planktonic foraminifera with pristine preservation still yield useful SST information (Pearson *et al.* 2001; Norris *et al.* 2002). Schrag, DePaolo & Richter (1995) note that at low latitudes, bottom water and pore fluid temperatures are cooler than surface water temperatures. Secondary calcite formed in the first few hundred metres of burial may have higher $\delta^{18}\text{O}$ than the primary calcite (see also Stoll & Schrag, 2000, p. 313), leading to underestimates of original SST. At mid- to high latitudes, primary $\delta^{18}\text{O}$ values for calcite formed in the mixed-layer near the ocean surface, are probably nearer the equilibrium values with cold pore water at the sea bottom (Schrag, DePaolo & Richter, 1995, p. 2271), so that SST estimates at these sites should more closely approach reality. In the small Pliocene dataset analysed here there is no clear trend between low latitude and greater calculated temperature difference from present (Fig. 7a,b); most SST estimates are simply cooler, up to and beyond 60°N . A provisional study of isotopic data from mid-Pliocene horizons older and younger than the Kaena Subchron also yield SST estimates cooler than at present (Fig. 12).

We have searched for the presence of diagenetic calcite by re-examining planktonic foraminifera at ODP sites 659, 704 and 925 in the Atlantic (Fig. 10). Although the tests of many of these foraminifera appear well preserved when viewed by light microscopy, when viewed by scanning electron microscopy the general preservation of specimens is less than pristine. Many specimens show veneers of calcite, often forming euhedral crystals on the test surface of *G. sacculifer*

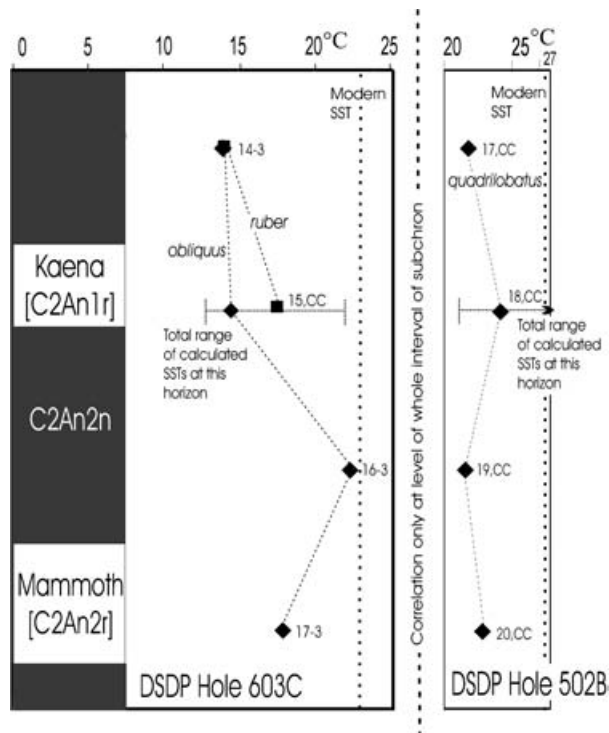


Figure 12. SST estimates through the Piacenzian (mid-Pliocene), from the isotopic signature of planktonic foraminifer calcite at DSDP holes 502B (Caribbean) and 603C (NW Atlantic) compared with modern SST at these sites. SST estimates are cooler than at present at both sites, though the degree of difference from present SST varies. Symbols against SST estimates (e.g. 17–3) indicate the core number for the source of the isotope data. The calculations use the Zachos, Stott & Lohmann (1994) equation to derive $\delta^{18}\text{O}_{\text{sw}}$. Note that only one isotopic datum is available for each subchron: in the Kaena Subchron the data for the two sites probably lie near the base of that interval; for the other isotopic data, the horizons may lie at any level within their subchron.

(Fig. 10a–c,e,g). In many cases these structures may be gametogenic (see Bé, 1980), but they may also represent secondary calcite formed after the foraminifer tests reached the sea bottom. Specimens of *G. sacculifer*, *G. bulloides* and *N. pachyderma* also show features that suggest fine-scale recrystallization of the test surface (Fig. 10h,k,l,m). It is possible to estimate the effects of calcite formed in sea bottom pore waters on the temperature signature of the foraminifer calcite using a simple mass balance equation:

$$\delta^{18}\text{O}_{\text{total}} = X\delta^{18}\text{O}_{\text{secondary}} + Y\delta^{18}\text{O}_{\text{primary}} \quad (8)$$

where $\delta^{18}\text{O}_{\text{total}}$ is the $\delta^{18}\text{O}$ of the primary foraminifer shell and the secondary calcite, $\delta^{18}\text{O}_{\text{secondary}}$ is the $\delta^{18}\text{O}$ of the secondary calcite formed in sea bottom pore waters, $\delta^{18}\text{O}_{\text{primary}}$ is the original $\delta^{18}\text{O}$ of the foraminifer shell calcite, X is the amount of secondary calcite (with $0 \leq X \leq 0.5$; the probable range of diagenetic overprint is up to 50% according to Pearson *et al.* 2001, and Pearson, Ditchfield & Shackleton, 2002), and Y is the amount of primary foraminifer calcite.

With

$$X + Y = 1$$

we can rewrite equation 8:

$$\delta^{18}\text{O}_{\text{primary}} = \frac{\delta^{18}\text{O}_{\text{total}} - X\delta^{18}\text{O}_{\text{secondary}}}{1 - X}$$

Values for $\delta^{18}\text{O}_{\text{secondary}}$ are estimated from the $\delta^{18}\text{O}$ of benthic foraminifer calcite (using the adjustment factors of Shackleton, Hall & Boersma, 1984). Thus, at tropical ODP hole 925B, specimens of *G. sacculifer* yielding $\delta^{18}\text{O}$ values of -1.72‰ (Fig. 4) require a correction for a little over 10% secondary calcite to produce a SST estimate similar to modern SST at this site. This assumes calcite formed in bottom waters with a $\delta^{18}\text{O}$ value of about 3‰ (see Billups, Ravelo & Zachos, 1997). However, the degree of calcite overprint may be much smaller than this, as some of the temperature offset will be due to calcite formed deep within, or below the mixed layer during the life of the foraminifer (e.g. gametogenic calcite; see Section 4.d, above).

Calcite formed in sea bottom pore waters may be less of an influencing factor in the temperature offset at higher latitudes, as the $\delta^{18}\text{O}$ contrast between surface and bottom waters is reduced. At DSDP Site 606, where there is a marked contrast between SST estimates from the oxygen isotopic composition of specimens of *G. bulloides* ($\delta^{18}\text{O}$ of 1.05‰) and modern SST (see Fig. 4), a correction for about 50% secondary calcite would be required to shift the estimated SST to a value for modern spring temperatures; this assumes carbonate forming at the sea bottom will have $\delta^{18}\text{O}$ values of about 3.3‰, based on mid-Pliocene specimens of *Cibicoides wuellerstorfi* at this site (see Keigwin, 1987). This degree of calcite overprint might be considered unlikely (see Zachos *et al.* 2002, Pearson *et al.* 2001, and Pearson, Ditchfield & Shackleton, 2002 for discussion), and other factors, in this case probably ecology (see Section 4.d), will have contributed to the cooler sea temperature estimates from *G. bulloides* at this site.

One site, ODP Hole 659A (see Fig. 7a,b) shows a range of SST estimates for the interval of the Kaena Subchron with maximum values exceeding the present, but minimum values much cooler than at present (Fig. 4). It will have been influenced by changes in the position of the cool Canary Current off the west coast of Africa. Marlow *et al.* (2000) also report a decline in SSTs between the mid-Pliocene and Quaternary interglacials at ODP Site 958 off the northwest coast of Africa. Some of the wide SST variation at ODP Site 659 will also relate to the variation of estimated $\delta^{18}\text{O}_{\text{sw}}$, which exceeds 1‰ (Fig. 8). Cool SST estimates at this site (some as low as 16.8°C, see Fig. 4) are probably also influenced by secondary calcite overgrowths on the tests of *G. sacculifer* (Fig. 10c,g).

Pearson *et al.* (2001, p. 485) inferred that stable isotope data from planktonic foraminifer tests preserved in carbonate oozes and chalks may be suspect, while material from clay-rich sites may be better preserved. At several of the Atlantic Ocean sites studied here (DSDP 516A, 517, 606), where the planktonic foraminifera were sourced from oozes, SST estimates are indeed cooler than those estimated by PRISM (Fig. 4). Also, planktonic foraminifer material from calcareous oozes at ODP sites 659, 704 and 925 is not pristine (Fig. 10). At one site (DSDP Hole 502B) in the Kaena Subchron, where SST estimates from oxygen isotopes are similar to that of PRISM (Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999), the lithology does comprise calcareous marls (Fig. 3b). Nevertheless, sites with clay-rich lithology also yield oxygen isotopic SST estimates much lower than PRISM (e.g. DSDP Hole 603C), so this does not appear to form a consistent pattern in our mid-Pliocene dataset.

5. Conclusions

(1) Oxygen isotope data from planktonic foraminifer tests at nine DSDP/ODP sites in the interval of the Kaena Subchron (3.12–3.05 Ma), when climatic conditions are interpreted to be warmer than at present, produce estimates of SSTs generally cooler than at present for the Atlantic Ocean through a present latitudinal range of 69.25° N to 46.88° S.

(2) Cooler SSTs contrast with fossil assemblage-based interpretation of SSTs by the PRISM Group for the mid-Pliocene 'Time Slab' (3.29–2.97 Ma; Dowsett, Barron & Poore, 1996; Dowsett *et al.* 1999) and with SST predictions from a coupled ocean–atmosphere GCM for the same time interval.

(3) The mismatch between estimates may highlight problems assessing SSTs from fossil assemblages and inaccurate determination of $\delta^{18}\text{O}_{\text{sw}}$ at some sites. However, the dominantly cool SST estimates from the $\delta^{18}\text{O}$ data are best explained by: (a) the effects of calcite formed near the base of, or below the ocean mixed-layer during the life of the foraminifera (particularly the presence of gametogenic calcite); and (b) taphonomic processes including secondary calcite (with higher $\delta^{18}\text{O}$) formed in cool sea bottom pore waters and especially important in tropical and sub-tropical sites.

(4) These results suggest that reconstruction of an accurate mid-Pliocene SST dataset required for General Circulation Models, with the existing published DSDP/ODP oxygen isotope data, requires a detailed re-assessment of taphonomy at many sites.

(5) The analysis also suggests that methods of estimating Pliocene $\delta^{18}\text{O}_{\text{sw}}$ need to be greatly improved, before more accurate estimates of SST can be produced for ancient time slices.

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