

Supplementary information for Quantifying Sea Surface Temperature Ranges of the Arabian Sea for the past 20,000 years, by Gerald Ganssen, Frank Peeters, Brett Metcalfe, Pallavi Anand, Simon Jung, Dick Kroon and Geert-Jan Brummer.

I. Outlier screening in oxygen isotope Individual Specimens Analyses:

In the study presented, Individual Specimen Analyses (ISA) oxygen isotope data are used to infer a range of calcification temperatures for a given species. It is generally known that the range is particularly sensitive to outliers, as it is defined by subtracting the observed/measured maximum from the minimum value, and therefore critically depends only on the two most extreme values. Since the resulting range of oxygen isotope ISA values is important for our conclusions, we consider it necessary to give special attention to this aspect of the data-analysis. We have compared different methods for outlier detection, and the impact of these analyses on the extreme values.

Various methods or approaches exist to screen for outliers, that is data points having an anomalous value. First, one could test or assume the data are normally distributed and label extreme observations based on the mean value \pm a range depending on the variance. Second, one does not (want to) make the assumption that the data are normally distributed, and uses methods that do not require this assumption. In addition to both methods one could follow two different approaches again; either one excludes consistently a few data values (e.g. based on a given percentile) in the tails of the distribution, or only exclude extreme values in case there is a firm basis for this. One cannot state a priori which of these methods is the best to be applied for the present study, and therefore we compare different approaches to see what would be the impact of the different methods.

Four different approaches defining the total $\delta^{18}O$ ranges and associated calcification temperature ranges are compared. The approaches we investigated are:

- 1). Ranges resulting from the raw data values;
- 2). Ranges resulting from excluding data outside the mean value $\pm 2.58 \times S.D.$, $S.D.$ being the standard deviation of the data;
- 3). Ranges resulting from excluding values using the Inter Quartile Range (IQR) of the data; i.e. outside the range $[Q1 - k \times IQR, Q3 + k \times IQR]$ in which $IQR = Q3 - Q1$, and k a given positive number often chosen to be 1.5 by commonly used software packages;
- 4). Ranges resulting from excluding values using the Median Absolute Deviation (MAD) of the data; i.e. outside the range $[M - k \times MAD; M + k \times MAD]$. Since for a normal distribution it can be shown that the standard deviation of the data equals $1.4826 \times MAD$, we will use $k = 3.8189$ for the detection of anomalous values. Hence we exclude data outside the range $[M - 3.8189 \times MAD; M + 3.8189 \times MAD]$; M being the median of the data-set.

The results of the outlier screening approaches are tabulated in Supplementary Tables 1 and 2, and graphically represented in the Supplementary Figures below here. In summary, each different method identifies a different number of

outliers. Out of a total of 1410 measurements, Approaches 2, 3 and 4 yielded 10, 19 and 41 outliers respectively. All methods identify more outliers on the low temperature side (high d_{18O}) compared to the high temperature side.

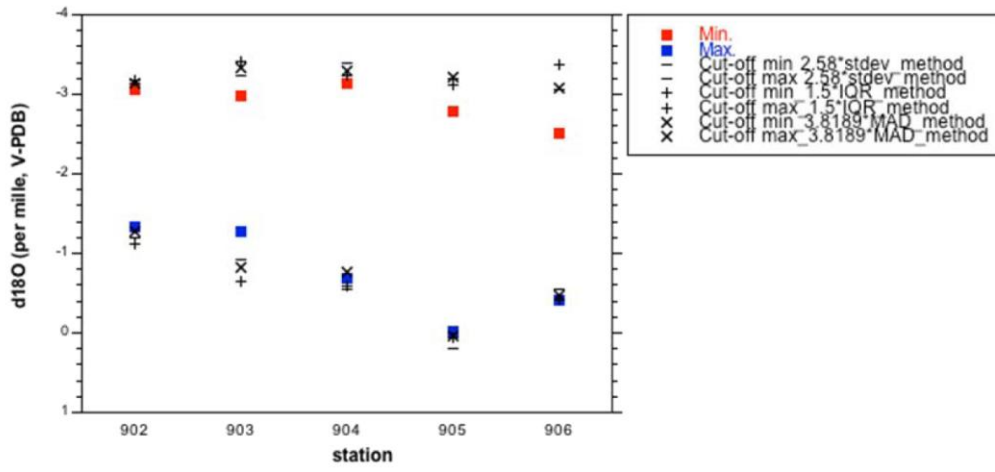
In case the data would be normally distributed, approaches 2 and 4 would theoretically remove about 1% of the data, while the IQR method with using $k=1.5$ theoretically remove about 0.74 % of the data. The results indicate that the data are not consistently normally distributed, and therefore approach 2 is not appropriate to use for identifying outliers.

This leaves us with the arbitrary choice of how strict we wish to be with removing anomalous data. Our choice here has been difficult, as it is hard to decide which of the two would be best. We have chosen to be conservative and remove as few data as possible. Knowing that this may lead to slightly reconstructed lower temperature minima, we could not find arguments to remove more data than strictly necessary.

II. Error.

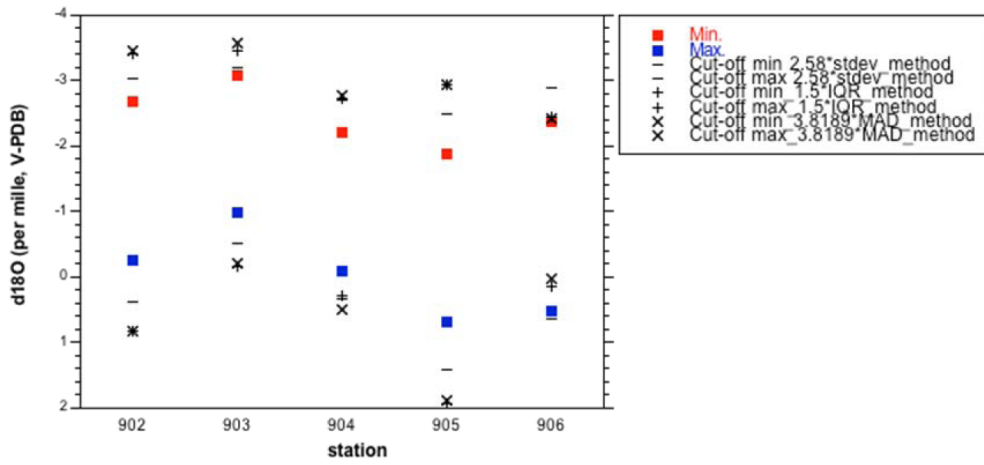
A minimum error that would be associated with the reconstructed calcification temperature maxima and minima depends on the errors associated with the Mg/Ca temperature as well as the error associated with the oxygen isotope measurement. The combined minimum standard error resulting from these two sources is estimate to be 1.1 °C. It needs to be stressed that, this is a minimum error, and that other potential sources of error e.g. small changes in the depth habitat of the species considered here cannot be reasonably quantified and have not been taken into account.

Comparison of outlier detection methods
***Globigerinoides ruber* box - core transect Somalia**
902B - 906B



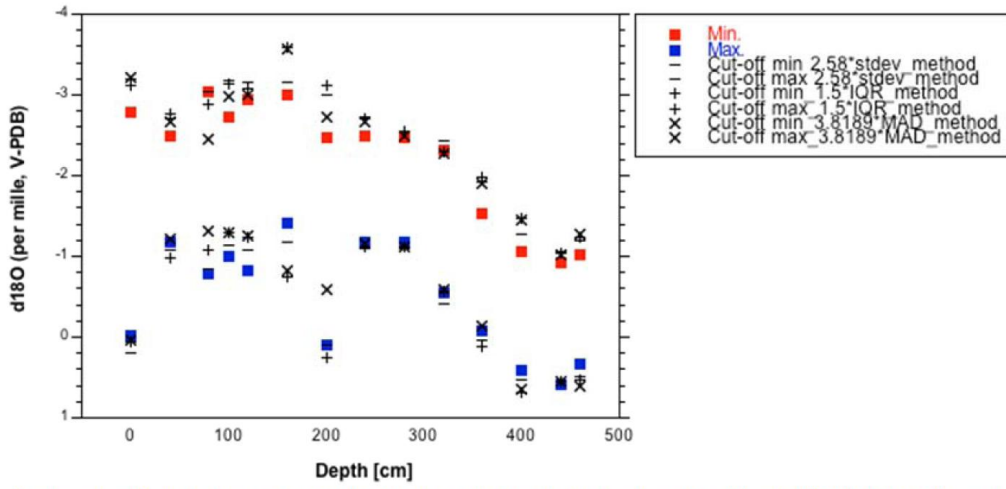
Supplementary Figure 1. Comparison of outlier detection methods applied to *G. ruber* (355 - 400 μm) d18O core tope data Somalia transect. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

Comparison of outlier detection methods
***Globigerina bulloides* box - core transect Somalia**
902B - 906B



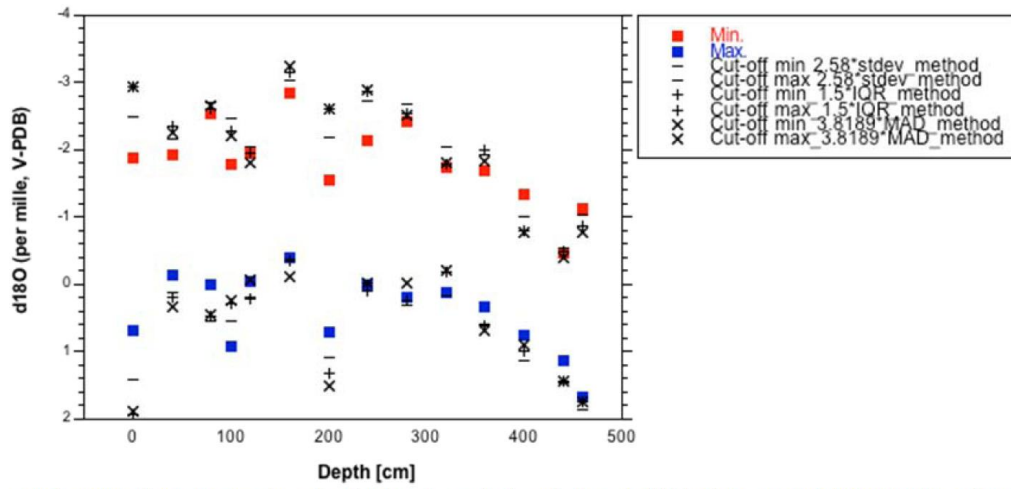
Supplementary Figure 2. Comparison of outlier detection methods applied to *G. bulloides*(300 - 355 μm) d18O core tope data Somalia transect. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

Comparison of outlier detection methods
Globigerinoides ruber - 905P



Supplementary Figure 3. Comparison of outlier detection methods applied to *G. ruber* (335 - 400 μm) d18O 905P data. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

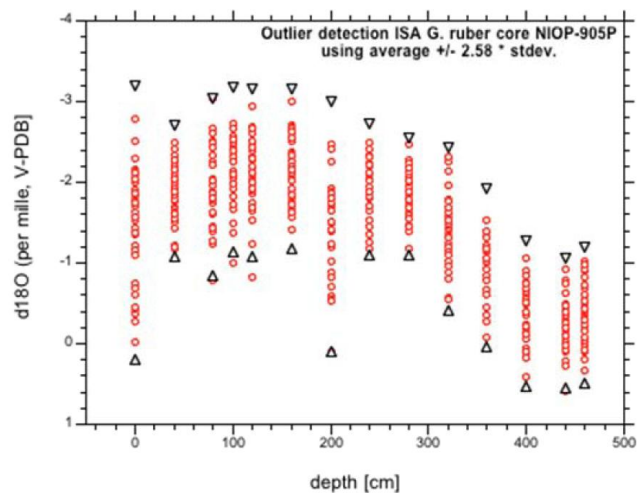
Comparison of outlier detection methods
Globigerina bulloides - 905P



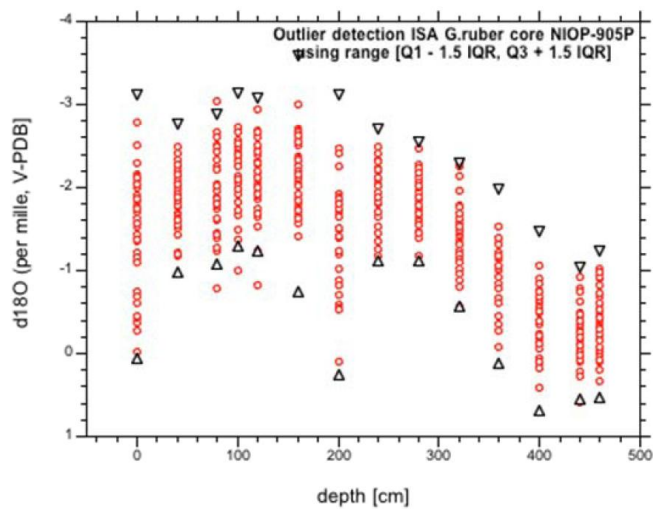
Supplementary Figure 4. Comparison of outlier detection methods applied to *G. boilloides* (300 - 355 μm) d18O 905P data. Observed minima and maxima in d18O are plotted as red and blue box symbols. Cut off levels for different outlier detection methods are given by black symbols.

Supplementary Figure 5. Visualisation of the four outlier correction methodologies for down core $\delta^{18}\text{O}$ range for (a-c) *G.ruber* (red circles) and (d-f) *G.bulloides* (blue circles), triangles represent cut off points. Method 1: Raw data range; Method 2: resulting from excluding data outside the mean value \pm two standard deviations; Method 3: from excluding values using the Inter Quartile Range (IQR) and Method 4: excluding values using the Median Absolute Deviation (MAD).

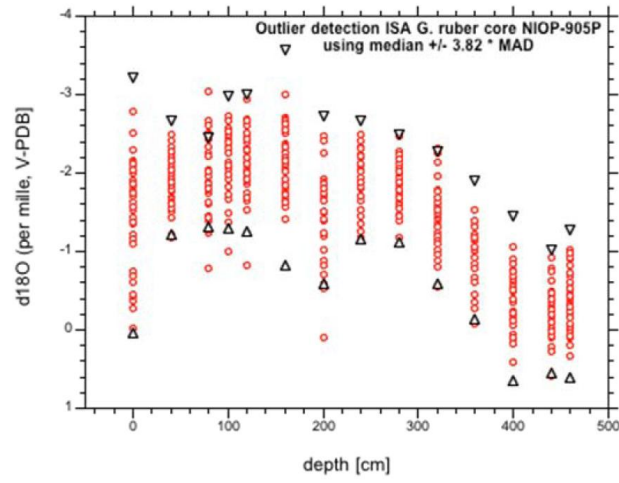
a)



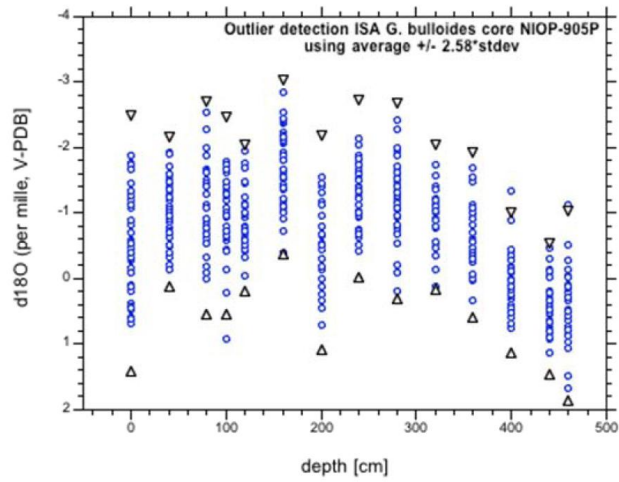
b)



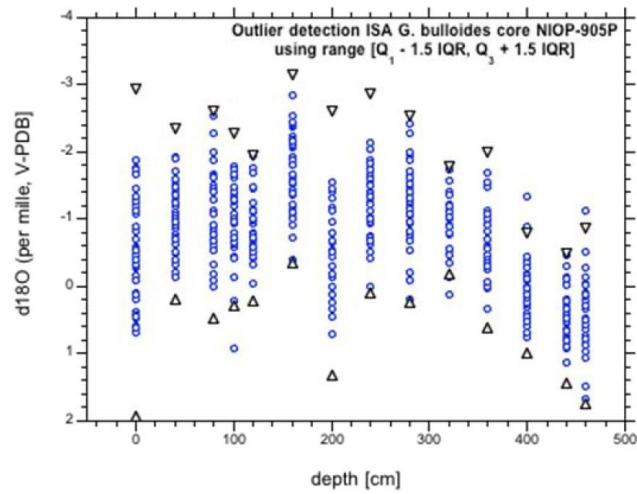
c)



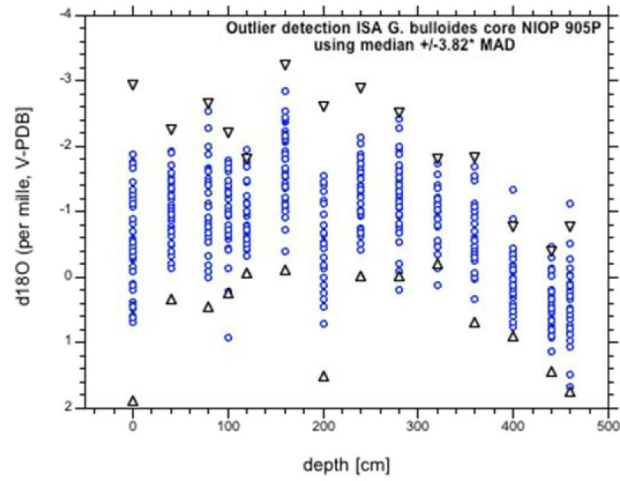
d)



e)

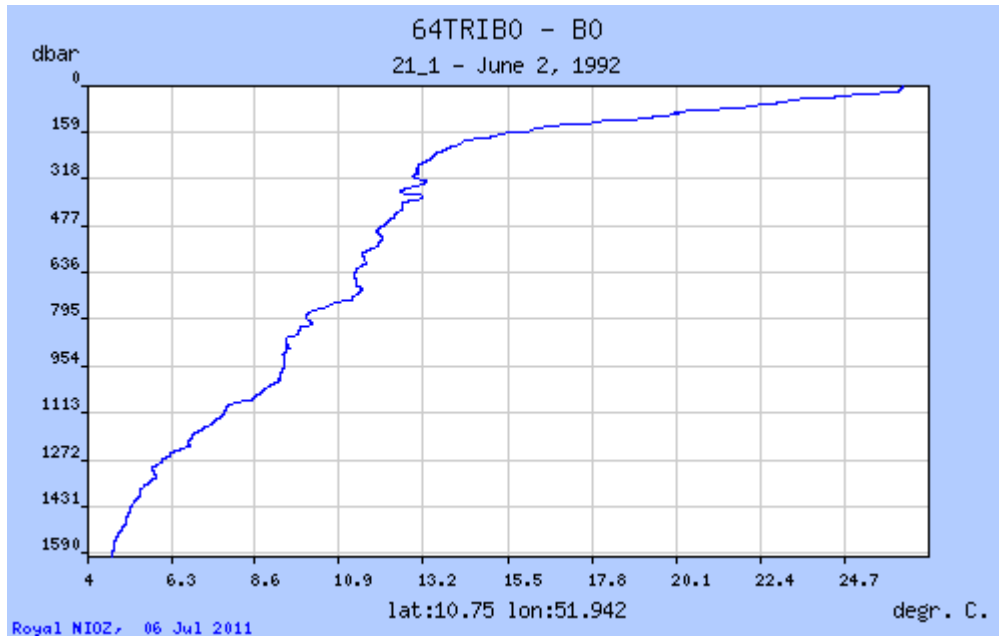


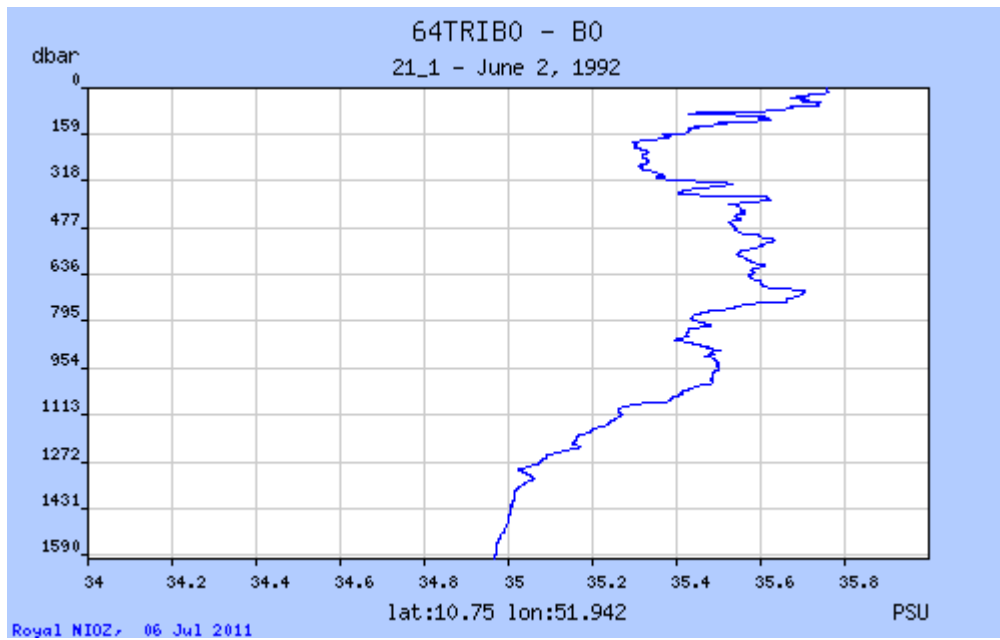
f)



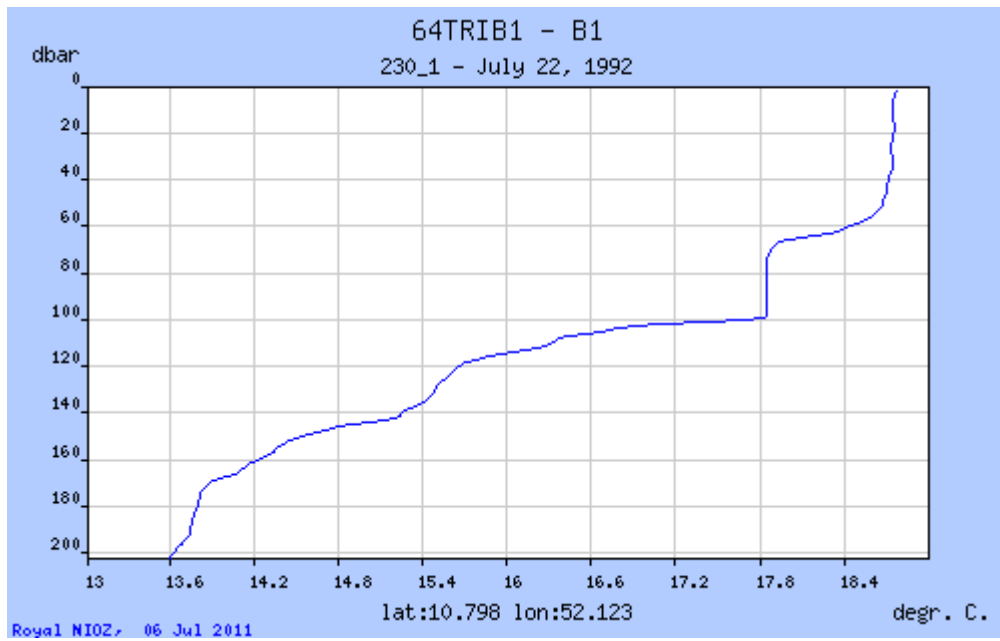
III. Temperature and Salinity Profiles

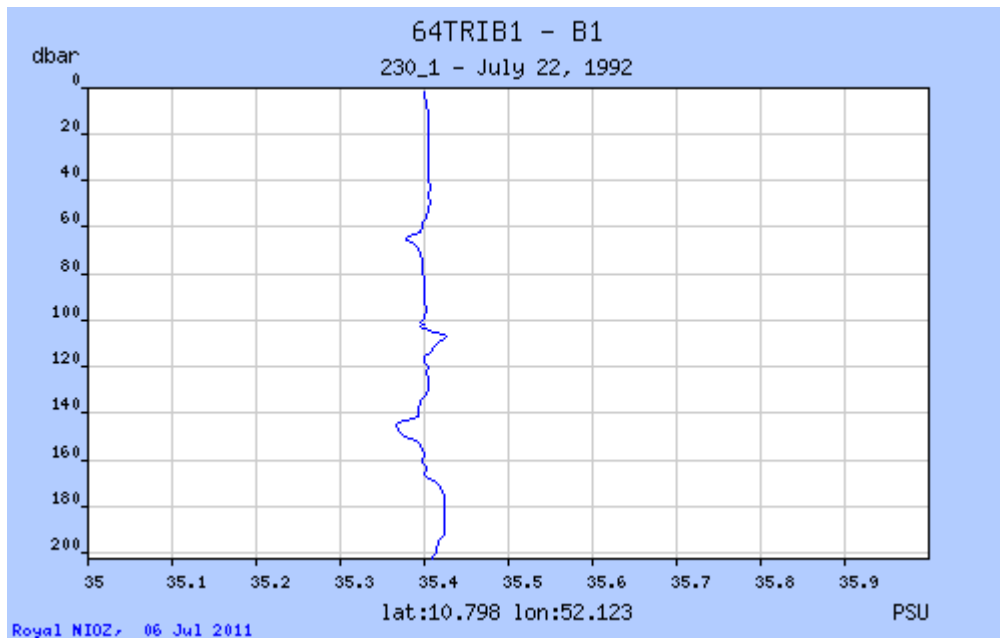
Temperature and salinity profiles at station 905 during pre-upwelling (June 1992), upwelling (July 1992) and winter monsoon (February 1993) conditions. Salinity range in the upper 500 m is within about 0.5 psu during all seasons.



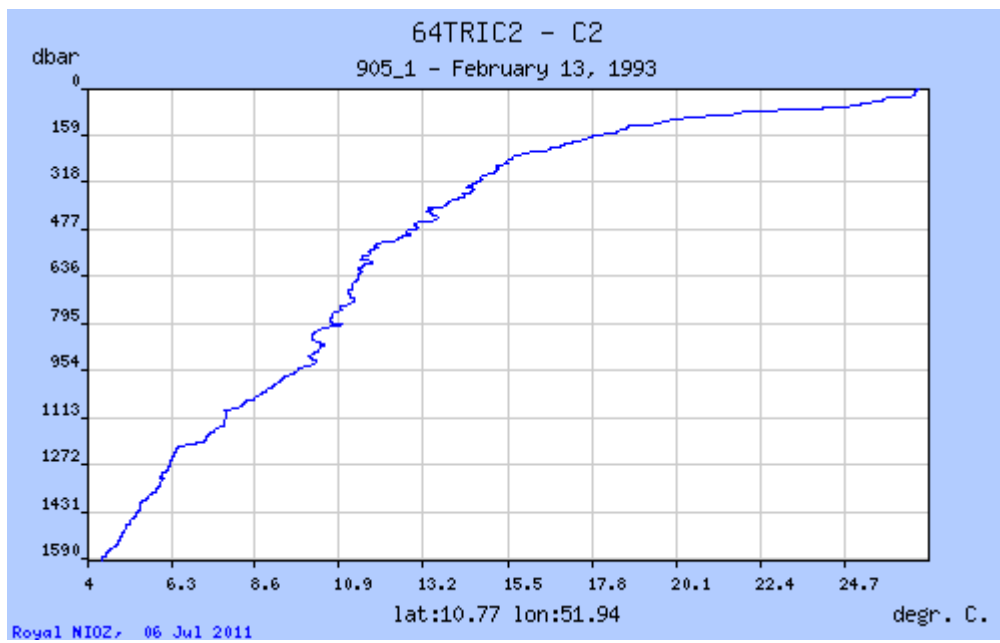


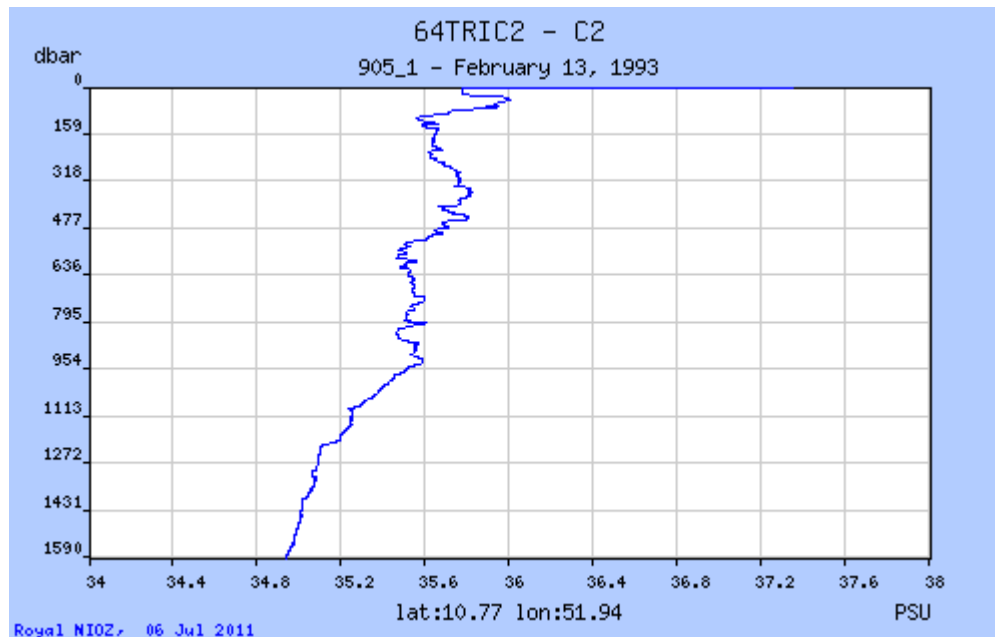
June 1992





July 1992





February 1993

IV. Sea Surface Temperature Profiles at location site

Sea surface temperature plots generated using the nomad live access server (LAS). Data was selected using the NOAA SST / optimum interpolation sea surface temperatures AVHRR method. The nine plots positioned half a degree surrounding the core-site 905. Whilst the time interval does not match the time interval apparent within the core, it shows the SST variability near the site on a daily scale – thus outlining the apparent range in temperatures that planktonic foraminifera would have likely seen during their lifetime. Depending on the depth of upwelling source water (Supplementary figure x) the temperature can vary considerably. For example upwelling of waters at 150m would produce sea surface temperatures of 15°C, whereas deeper upwelling (300m) would produce SST of 13°C.

Supplementary Table 2: Calcification temperatures, minima & maxima

core	core type	depth [m]	species	size fraction LL	size fraction UL	Mg/Ca_derived_temperature [°C]	T_min_all_data	T_max_all_data	T_min_OL_rem_2.58*SD	T_max_OL_rem_2.58*SD	T_min_OL_rem_IQR	T_max_OL_rem_IQR	T_min_OL_rem_MAD	T_max_OL_rem_MAD
902B	box	0.00	<i>Globigerinoides ruber</i>	355	400	26.02	22.2	30.1	22.2	30.1	22.2	30.1	22.2	30.1
903B	box	0.00	<i>Globigerinoides ruber</i>	355	400	25.71	22.1	29.8	22.1	29.8	22.1	29.8	22.1	29.8
904B	box	0.00	<i>Globigerinoides ruber</i>	355	400	25.90	20.0	31.2	20.0	31.2	20.0	31.2	21.2	31.0
905B	box	0.00	<i>Globigerinoides ruber</i>	355	400	24.71	18.0	30.6	18.0	30.6	18.0	30.6	18.0	30.6
906B	box	0.00	<i>Globigerinoides ruber</i>	355	400	24.47	18.2	27.6	20.7	27.4	18.2	27.6	20.7	27.4
907B	box	0.00	<i>Globigerinoides ruber</i>	355	400	25.63	22.6	28.8	22.6	28.8	22.6	28.8	22.6	28.8
905P	piston	0.40	<i>Globigerinoides ruber</i>	355	400	24.11	20.9	26.8	20.9	26.8	20.9	26.8	21.8	26.6
905P	piston	0.80	<i>Globigerinoides ruber</i>	355	400	25.39	20.2	30.4	22.1	30.2	22.2	28.7	23.1	27.8
905P	piston	1.00	<i>Globigerinoides ruber</i>	355	400									
905P	piston	1.20	<i>Globigerinoides ruber</i>	355	400	25.20	19.3	28.9	21.0	28.8	22.3	28.7	22.3	28.7
905P	piston	1.60	<i>Globigerinoides ruber</i>	355	400	24.91	21.5	28.7	21.5	28.7	21.5	28.7	21.5	28.7
905P	piston	2.00	<i>Globigerinoides ruber</i>	355	400	25.34	18.3	30.0	20.9	29.7	18.3	30.0	21.3	29.3
905P	piston	2.40	<i>Globigerinoides ruber</i>	355	400	25.48	22.2	28.1	22.2	28.1	22.2	28.1	22.2	28.1
905P	piston	2.80	<i>Globigerinoides ruber</i>	355	400	25.47	22.5	28.4	22.5	28.4	22.5	28.4	22.5	28.4
905P	piston	3.20	<i>Globigerinoides ruber</i>	300	400	25.74	21.8	29.9	21.8	29.9	22.9	29.5	22.9	29.5
905P	piston	3.60	<i>Globigerinoides ruber</i>	355	400	24.61	20.7	27.3	20.7	27.3	20.7	27.3	21.4	27.2
905P	piston	4.00	<i>Globigerinoides ruber</i>	355	400	23.85	20.3	27.0	20.3	27.0	20.3	27.0	20.3	27.0
905P	piston	4.40	<i>Globigerinoides ruber</i>	355	400	22.74	18.9	25.8	20.2	25.7	20.2	25.7	20.2	25.7
905P	piston	4.60	<i>Globigerinoides ruber</i>	355	400	22.94	19.8	26.0	19.8	26.0	19.8	26.0	19.8	26.0
902B	box	0.00	<i>Globigerina bulloides</i>	300	355									
903B	box	0.00	<i>Globigerina bulloides</i>	300	355	22.00	18.1	27.5	18.1	27.5	18.1	27.5	18.1	27.5
904B	box	0.00	<i>Globigerina bulloides</i>	300	355	21.43	16.5	26.1	16.5	26.1	16.5	26.1	16.5	26.1
905B	box	0.00	<i>Globigerina bulloides</i>	300	355	21.23	15.7	27.3	15.7	27.3	15.7	27.3	15.7	27.3
906B	box	0.00	<i>Globigerina bulloides</i>	300	355	20.25	12.8	26.0	12.8	26.0	14.0	25.5	15.5	25.1
907B	box	0.00	<i>Globigerina bulloides</i>	300	355	20.60	14.2	27.5	14.2	27.5	14.2	27.5	14.2	27.5
905P	piston	0.40	<i>Globigerina bulloides</i>	300	355	21.33	17.3	25.5	17.3	25.5	17.3	25.5	17.3	25.5
905P	piston	0.80	<i>Globigerina bulloides</i>	300	400	19.93	15.0	26.5	15.0	26.5	15.0	26.5	15.0	26.5
905P	piston	1.00	<i>Globigerina bulloides</i>	300	355									
905P	piston	1.20	<i>Globigerina bulloides</i>	300	400	20.82	16.8	25.5	16.8	25.5	17.0	24.8	18.1	24.7
905P	piston	1.60	<i>Globigerina bulloides</i>	355	400	20.56	14.6	25.7	14.6	25.7	14.6	25.7	14.6	25.7
905P	piston	2.00	<i>Globigerina bulloides</i>	300	355	21.46	15.7	26.0	15.7	26.0	15.7	26.0	15.7	26.0
905P	piston	2.40	<i>Globigerina bulloides</i>	300	355	21.37	15.1	24.9	16.9	24.7	15.1	24.9	16.9	24.7
905P	piston	2.80	<i>Globigerina bulloides</i>	300	355	20.80	14.6	26.4	14.6	26.4	14.6	26.4	15.7	26.3
905P	piston	3.20	<i>Globigerina bulloides</i>	300	355	22.29	17.4	25.9	17.4	25.9	19.3	25.5	19.3	25.5
905P	piston	3.60	<i>Globigerina bulloides</i>	300	400	20.34	15.8	25.0	15.8	25.0	15.8	25.0	15.8	25.0
905P	piston	4.00	<i>Globigerina bulloides</i>	300	355	19.74	16.6	26.1	16.8	24.2	16.9	22.3	16.9	22.3
905P	piston	4.40	<i>Globigerina bulloides</i>	300	355	18.55	15.5	22.8	15.5	22.8	15.5	22.8	15.6	22.2
905P	piston	4.60	<i>Globigerina bulloides</i>	300	355	19.95	14.2	26.9	14.5	24.4	14.5	24.4	14.5	24.4

