Q-Mode and R-Mode Factor Analysis in Quantitative Studies of Microfossils of the Late Quaternary in Sediments from the Brazilian Continental Margin

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Abstract *Q-mode and R-mode factor analysis in quantitative studies of microfossils of the late quaternary in sediments from the brazilian continental margin. In the present article Q and R-mode factor analyses were performed on quantitative data of coccolithophores and foraminifera from samples of the upper Quaternary of the Campos and Santos basins, using the software STATISTICA 7. The obtained factors attempt to explain the variation of taxa which can be attributed to the influence of certain environmental parameters, such as changes in the thermocline, nutricline, temperature and salinity among others. The employment of the two statistical techniques attempts to demonstrate the good potential of the quantitative study of microfossils applied to paleoceanography.*

Keywords *Calcareous nannoplankton, planktonic foraminifera, Q and R-mode factor analyses, Quaternary*

1. Introduction

The investigation of the composition of marine microfossil associations is an important tool in paleoclimatic and paleoceanographic reconstructions. Foraminifera tests and calcareous nannofossils are the widest calcareous microfossils employed for paleoceanographic purposes (CLIMAP, 1981; Toledo, 2000; Buccheri et al., 2002; Toledo et al., 2007).

Calcareous nannofossils are remains of a significant part of the phytoplankton in the marine realm and one of the main open ocean primary producers (Roth, 1994). Foraminifera represent one of the most ecologically important groups of marine heterotrophic protists (Gupta, 1999). Together they form a major sink for pelagic carbonate (Bradley, 1999). Their excellent preservation, global occurrence and high abundance in marine deep sea sediments are prime reasons for the extensive application in paleoceanographic and paleoclimatic studies.

Planktonic foraminifera and calcareous nannofossils distribution are influenced by a variation of physical and chemical parameters linked to oceanography such as: light, temperature, salinity, water stratification, turbidity and nutrient availability, as well as by biological parameters (Schmidt et al., 2003; Buccianti & Esposito, 2004). Such parameters vary temporally and geographically and can affect the structure of these microfossil associations. Consequently, quantitative and qualitative analyses of planktonic foraminifera and calcareous nannofossils assemblages allow both reconstruction of the climatic oscillations and detection of the ecological changes that strongly influenced the distribution of some species (Toledo et al., 1999; Toledo, 2000; Buccianti & Esposito, 2004).

Micropaleontological data are commonly expressed as relative abundances, for example percentages of a series of species in relation to the total fauna or flora. Multivariate statistical approach and numerical methods of data treatment are frequently applied in this kind of study due to the large number of variables (species) varying through several cases (samples). Its application is almost exclusively based on correlation or covariance matrices determined directly from the raw percentage (Kucera, 2003).

Factor analysis is a statistical approach used to analyze interrelationships among a large number of variables and to explain these variables in terms of their common underlying dimensions, called *factors*. The factor analysis involves finding a way of condensing the information contained in a number of original variables into a smaller set of dimensions with minimum loss of information.

In the light of the above considerations, the changes shown by abundance of planktonic foraminifera, recorded in core SAN-76, and calcareous nannofossils recorded in core PC-01, both sampled in the Brazilian Continental Margin, were examined. We attempt here to compare the application of two factor analytic data modes – Q-mode factor analysis and R-mode factor analysis – applied to marine micropaleontological data, concerning which is more suitable for paleoceanographic studies. The difference between Q-mode and R-mode is that the later seeks to cluster variables on a set of cases, at a given point in time, while Q-mode clusters the cases rather than the variables, establishing the factional composition of a group on a set of issues.

The application of these two techniques on different groups of organisms considered was also evaluated.

2. Methods

The PC-01 piston core, 495 cm long (50 samples), was recovered from Campos Basin (22°23'S, 40°18'W) at 990 m water depth and used for Quaternary calcareous nannofossils analysis. The SAN-76 piston core, 419 cm long (43 samples), was recovered from Santos Basin (24°44'S, 42°30'W) at 1682 m water depth and used for Quaternary planktonic foraminifera analysis. The piston cores were sampled at intervals of 10 cm. Microfossils quantitative analysis were performed by counting 300 coccoliths as well as 300 planktonic foraminifera tests. According to Roth (1994) and Bown & Young (1998) 300 counts assures the presence of a taxon whose relative abundance was 1% in the total population, at the 95% confidence level. Planktonic foraminifera oxygen isotopic data, ^{14}C (AMS) radiometric dating performed on 2 selected samples (SAN-76) along with previous biostratigraphic zonation (Toledo, 2000) provided the stratigraphic framework which gave support to downcore interpretations.

The species absolute number for each sediment sample was transformed into relative abundance, which then provided a data matrix. Data matrices were the main input to the statistical procedure. The STATISTICA for Windows program, version 7.0 was used for the factor analysis.

2.1. Statistical procedure

By generating a Q-mode and a R-mode correlation matrix it is possible to assert correlations between samples and species, respectively. This matrix is important to verify technique suitability, since factor analysis is recommended only when a significant number of correlations is superior to 0.3 (Gouvêa, 2003). To extract factors from the data sets the Principal Components Analysis method, the most common form of factor analysis, was chosen. The criteria considered to determine the number of factors to be retained for further analysis was suggested by Harman (1976): the number of factors should be between 1/6 and 1/3 of the variables number, or those factors whose eigenvalue was greater than 1. Subsequently, the factor loadings, which represent the correlation coefficients between the variables and the factors, were considered. It is important to find how much of the variance in such variable is explained by that factor. Factor loadings are the basis for imputing a label to the different factors. To obtain more interpretable results the output solution was rotated by the Varimax method.

3. Results

Most of correlation coefficients were greater than 0.3 for both Q- mode and R-mode techniques, indicating the data sets were appropriate for factor analysis.

3.1. Pc-01 (calcareous nannofossil based)

3.1.1. Q-mode factor analysis

Two factors were retained. Together they explain 95.28% of the total variance of the calcareous nannofossil data set. Factor 1 was the most important responding for 93.02% while factor 2 elucidates only 2.26% of total variance (Table 1). Once rotating the solution, factor loadings allowed finding the key samples for each factor , only values greater than 0.60 were considered (Figueiredo, 1996). The results of Q-mode factor analysis are given by two graphs (Figures 1 and 2). In the first

Table 1 – PC-01 Q-mode factors and their eigenvalues, variance and cumulative variance

Factor	Eigenvalue	Variance(%)	Cumulative Variance
1	46,51361	93,02722	93,0272
2	1,13109	2,26217	95,2894
3	0,85505	1,71010	96,9995
4	0,70185	1,40370	98,4032
5	0,38131	0,76262	99,1658
6	0,20468	0,40935	99,5752
7	0,13415	0,26830	99,8435
8	0,03563	0,07127	99,9147
9	0,02373	0,04745	99,9622
10	0,01180	0,02359	99,9858
11	0,00711	0,01422	100,0000

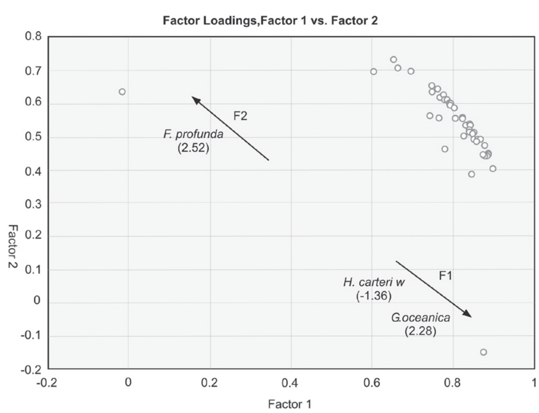


Figure 1 – PC-01 Q-mode factor 1 and 2 correlation. Plots represent samples and species numerical data refer to Table 4

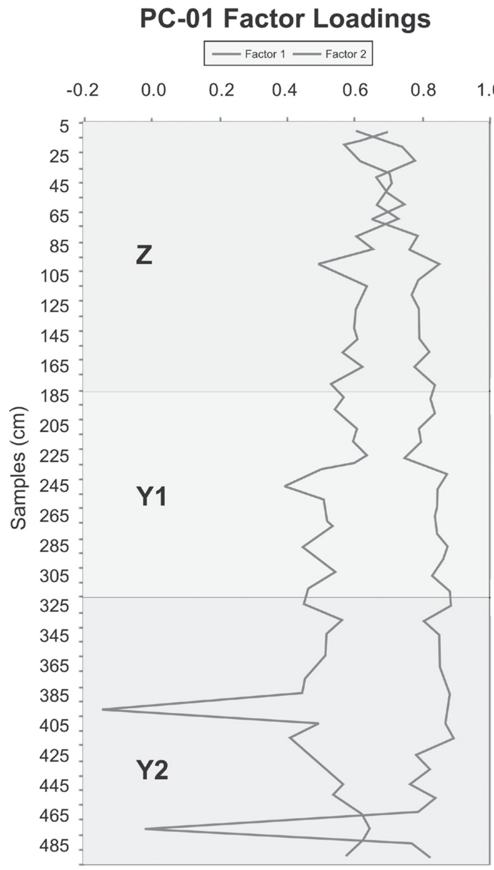


Figure 2 – PC-01 Q-mode factor 1 and 2 loadings and planktonic foraminifera determined zones Z (interglacial), Y1 and Y2 (glacial)

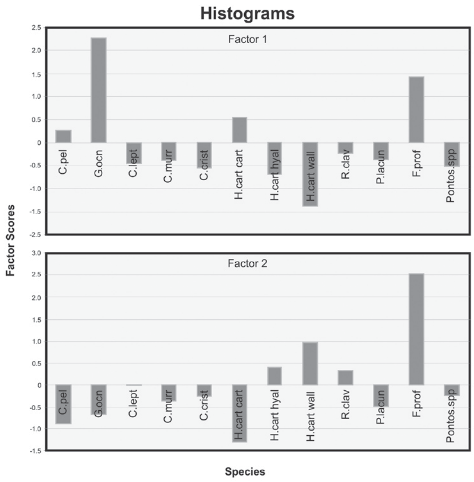
graph (Fig.1), PC-01 samples distribution according to their factor loadings as well as their trends are shown. Major factor scores are also reported (*Florisphaera profunda*, *Gephyrocapsa oceanica* and *Helicosphaera sp.*). In the second graph (Fig.2), factor loadings of both the factors are plotted throughout the core, within planktonic foraminifera zones Y2, Y1 (glacial) and Z (interglacial) are indicated. The factor contribution (factor scores) to each species is demonstrated in table 2 and figure 3 (histograms).

3.1.2. R-mode factor analysis

Explaining 66.32% of the total variance of the calcareous nannofossils data set, four factors were considered in this analysis. Factor 1 denoted 27.27% of total variance, followed by 15.96% (factor 2), 11.87% (factor 3) and 11.21% (factor 4) (Table 3). The positive and negative higher loadings of calcareous nannofossils species given by each

Table 2 – PC-01 Q-mode factor scores

	Factor 1	Factor 2
C. pelagicus	0,27847	-0,88416
G. oceanica	2,28384	-0,66537
C. leptoporus	-0,44095	0,00033
C. murrayi	-0,37657	-0,38970
C. cristatus	-0,53419	-0,24565
H. carteri var.carteri	0,55436	-1,28724
H. carteri var.hyalina	-0,66931	0,40111
H. carteri var.wallichii	-1,36503	0,98580
R. clavigera	-0,22248	0,31391
P. lacunosa	-0,38871	-0,48826
F. profunda	1,40932	2,52329
Pontosphaera spp.	-0,52875	-0,26405



Key: C.pel, Coccolithus pelagicus; G.ocn, Gephyrocapsa oceanica; C.lept, Calcidiscus leptoporus; C.murr, Calciosolenia murray; C.crist, Ceratolithus cristatus; H.cart cart, Helicosphaera carteri carteri; H.cart hyal, Helicosphaera carteri hyalina; H.cart wall, Helicosphaera carteri wallichi; R.clav, Rhabdosphaera clavigera; P.lacun, Pseudoemiliania lacunosa; F.prof, Florisphaera profunda and Pontos.spp, Pontosphaera spp.

Figure 3 – PC-01 Q-mode factor 1 and 2 histograms indicating factor scores of the taxa analysed

retained factor were used for factors interpretations and labels. Figure 4 illustrates factor scores of each factor throughout the core with planktonic foraminifera zones Y2, Y1 and Z indicated.

Table 3 – PC-01 R-mode factors and their eigenvalues, variance and cumulative variance

Factor	Eigenvalue	Variance (%)	Cumulative Variance
1	3,272724	27,27270	27,2727
2	1,915284	15,96070	43,2334
3	1,424801	11,87334	55,1067
4	1,346172	11,21810	66,3249
5	1,031411	8,59509	74,9199
6	0,832165	6,93471	81,8547

3.2. SAN-76 (planktonic foraminifera based)

3.2.1. Q-mode factor analysis

Among 34 extracted factors, only two of them were retained for further paleoenvironmental interpretation. Factor 1 alone explained 93.72% of the total variance of the planktonic foraminifera data set, while factor 2 responded for 3.61% (Table 4). The results of Q-mode factor analysis are given by figures 5 and 6. The later correlates factor loadings, oxygen isotopic data and biozones Y and Z throughout SAN-76. Factor 1 and factor 2 contributions (factor scores) to each foraminifera species is demonstrated in figure 7 (histograms), outstand values were referred in figure 5 (*Globigerinba bulloides, Globigerinoides ruber, Globigerinita glutinata* and *Globorotalia inflata*).

Table 4 – SAN-76 Q-mode factors and their eigenvalues, variance and cumulative variance

Factor	Eigenvalue	Variance (%)	Cumulative Variance
1	40,29992	93,72074	93,7207
2	1,55204	3,60940	97,3301
3	0,45800	1,06511	98,3952

3.2.2. R-mode factor analysis

Eleven factors were retained from 35 extracted. They accounted for 76.08% of the total variance of the planktonic foraminifera data set (Table 5). Figure 8 reported factors influence throughout the core (factor scores), plotted together with planktonic foraminifera zones Y and Z and oxygen isotopic data.

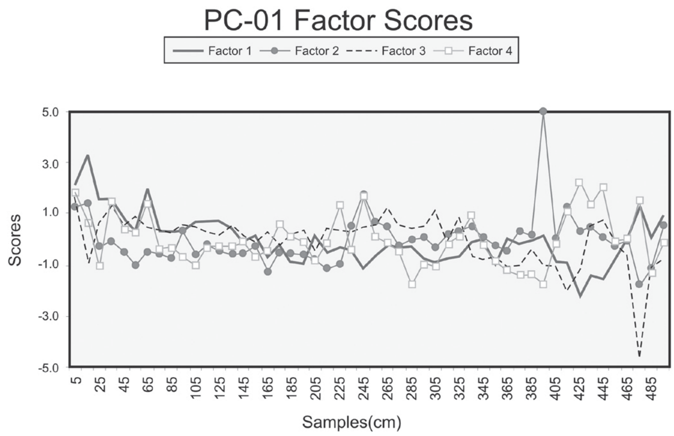


Figure 4 – PC-01 R-mode factor 1, 2, 3 and 4 scores and planktonic foraminifera determined zones Z (interglacial), Y1 and Y2 (glacial)

4. Discussion

4.1. Q-mode PC-01

According to factor loadings most of the PC-01 sediment samples were strongly influenced by factor 1 (Figure 1), however 17 samples were in agreement with factor 2: 5 cm, 25 to 85 cm, 115 cm, 125 cm, 145 cm, 165 cm, 205 cm, 225 cm and 465 to 485 cm. As reported in figure 1 higher factor score for factor 1 was related to *G. oceanica* (2.28) while *F. profunda* (2.52) associated to factor 2. These values indicate factor 1 had influenced *G. oceanica* temporal distribution along PC-01 and factor 2 controlled *F. profunda*. *G. oceanica* tend to be very abundant in nutrient-rich waters (Brand, 1994), this species exhibits preference for neritic environments by reducing its abundance with depth. At the same time *F. profunda* is known as a pelagic deep-living species increasing its abundance in proportion to water depth (Okada, 1992). The nutrient availability is controlled by the depth of the nutricline, which can be monitored by the abundance of *F. profunda* (Molfino & McIntyre, 1990; Kinkel et al., 2000). Taking these ecological preferences into account, factor 1 was interpreted as surface water productivity whereas factor 2 was labeled as nutricline depth variation. In accordance with figure 2 surface water productivity (factor 1) was more prominent during glacial interval (biozone Y2 and Y1). Conversely, through interglacial interval (biozone Z) nutricline depth (factor 2) seems to display a significant role.

4.2. Q-mode SAN-76

Explaining 97.33% of the total variance, the two factors considered in this analysis are represented in figure 5. Following PC-01 pattern the majority of SAN-76 samples are characterized by the dominant factor 1, but ten of them are influenced by the second factor: 241 cm, 342 cm, 353 cm, 364 cm, 403 cm, 408 cm, 412 cm, 416 cm and 419 cm, which are clustered along glacial interval (biozone Y) (Figure 6). Regardless of its dominance throughout the core, factor 1 has shown its greatest values during interglacial interval (biozone Z). According to factors contribution (factor scores) on each species it is possible to verify that *G. ruber* was chiefly influenced by factor 1 followed by *G. glutinata*, whilst *G. bulloides* and *G. inflata* (minor) were addressed to factor 2 (Figure 7). Thus, as the former two species are abundant in the ocean mixed layer (Fairbanks et al. 1982; Ravelo et al., 1990; Andreasen & Ravelo, 1997), we interpreted factor 1 as mixed layer. On the other hand *G. bulloides* and *G. inflata* are more common in cold and productive waters (Hemleben et al., 1989; Hilbretch, 1996; Toledo, 2000). Therefore, factor 2 can be designed as surface temperature or productivity, which is consistent with glacial conditions.

4.3. R-mode PC-01

The first factor extracted by this analysis was strongly associated to *Coccolithus pelagicus* (negative

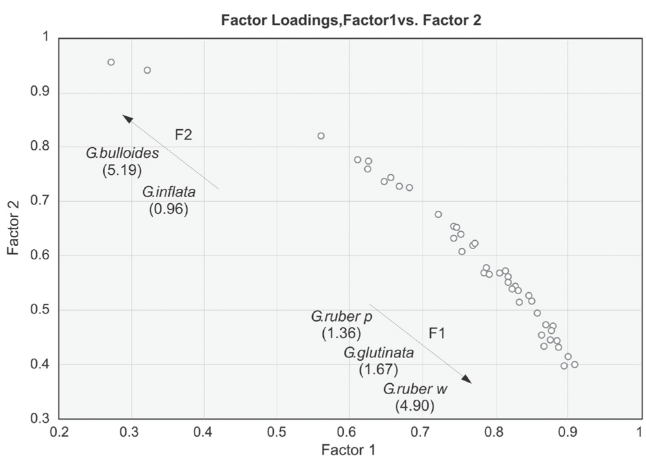


Figure 5 – SAN-76 Q-mode factor 1 and 2 correlation. Plots represent samples and species numerical data refer to Table 9

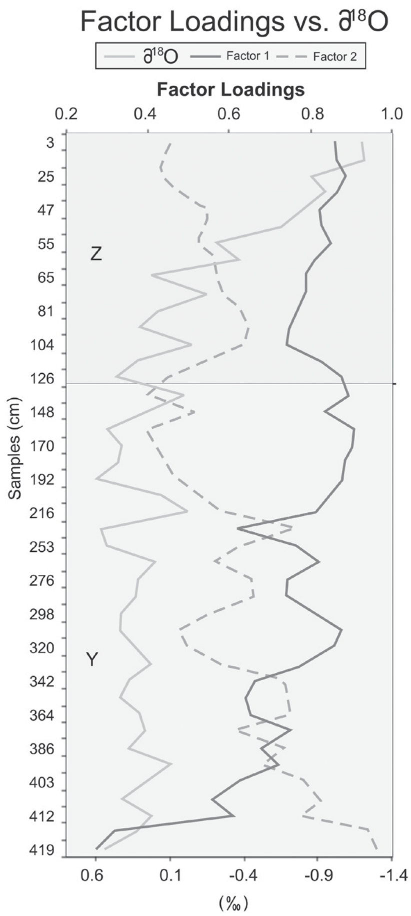


Figure 6 – SAN-76 Q-mode factor 1 and 2 loadings, oxygen isotopic curve and planktonic foraminifera determined zones Z (interglacial) and Y (glacial)

loading), *Ceratolithus cristatus, Helicosphaera carteri var. hyalina* and *Pontosphaera spp.* According to factor scores (Figure 4) factor 1 begins to be distinctive only in biozone Z (about 145 cm). Factor 2 was linked to glacial samples and to species like *Helicosphaera carteri var. carteri* and *F. profunda* (negatively); factor 3 showed correspondence to *H. carteri var. wallichii, Pseudoemiliania lacunosa* (negative loadings) and *Rabdosphaera clavigera*, this factor seems to be related to two distinct biozones (Y1 and Z), which correspond, respectively, to colder glacial and interglacial. Finally the fourth factor retained showed an oscillating behavior, being present over the three biozones. This factor was chiefly associated to *G. oceanica* and *C. murrayi* (negative loadings). Bearing it in mind we could assert that factor 1 is related to temperature, since *C. pelagicus* prefers cold waters (Brand, 1994) and *C. cristatus* increases its relative abundance in warm waters (Buccheri et

Table 5 – SAN-76 R-mode factors and their eigenvalues, variance and cumulative variance

Factor	Eigenvalue	Variance (%)	Cumulative Variance
1	7,334675	19,82344	19,8234
2	3,907353	10,56041	30,3839
3	2,861672	7,73425	38,1181
4	2,396459	6,47692	44,5950
5	2,226350	6,01716	50,6122
6	1,968353	5,31987	55,9321
7	1,732653	4,68285	60,6149
8	1,559941	4,21606	64,8310
9	1,511972	4,08641	68,9174
10	1,377453	3,72285	72,6402
11	1,272845	3,44012	76,0803
12	1,129443	3,05255	79,1329
13	0,968568	2,61775	81,7506

al., 2002); factor 2 can be a nutricline depth indication due to the *F. profunda* relationship; factor 3 is suggested to be related to light penetration given that *R. clavigera* is favored by high intensity levels at ocean surface, this species also seems to decrease its abundance in proportion to water depth (Okada & Honjo,1973), and lastly *G. oceanica* and *C. murrayi* negative loadings related to factor 4 should be a sign of low surface productivity or high salinity waters since *Gephyrocapsa spp.* are related to reduced water salinity and eutrophic environments (Okada, 1992; Buccheri et al., 2002) and *C. murrayi* seems to have an affinity for coastal conditions (Andruleit et al., 2004).

4.4. R-mode SAN-76

Although 11 factors were statistically significant, only five of them were used for environmental inference. The other six factors were not interpreted because ecological preferences of related species are poorly understood. The factors taken into account were 1, 2, 3, 5 and 9. *Globigerina falconensis* and *Globorotalia menardii* showed high correlation to factor 1, which was labelled as thermocline influence as these species are related to temperatures at 200m and warm sea surface temperatures, respectively (Hilbrecht, 1996). Factor 2 addressed negative loadings to *Globigerina bulloides* and *Neogloboquadrina dutertrei* which can be related to colder and productive temperate waters while factor 3 was interpreted as water column stratification in view of the fact that *Globorotalia truncatulinoides* and *Pulleniatina obliquiloculata* are deep-dwelling species which ascend to shallower

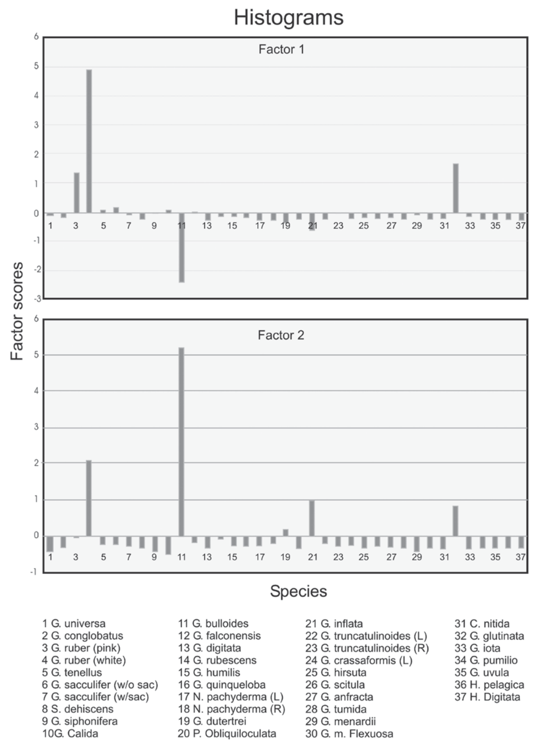


Figure 7 – SAN-76 Q-mode factor 1 and 2 histograms indicating factor scores of the taxa analysed

depths during their reproduction period in winter, when the vertical density gradient is reduced. *G. ruber* (pink) and *G. inflata* were also associated to factor 3 to stratified waters (Hilbrecht, *op.cit.*). As a consequence of *G. truncatulinoides* and *G. inflata* tolerance to little variation in salinity, factor 3 can be related to salinity as well. Both forms of *Globigerinoides sacculifer,* which have a preference for the mixed layer (Fairbanks et al. 1982; Ravelo et al., 1990; Andreasen e Ravelo, 1997), were the greatest contribution to factor 5. Thus it was interpreted as mixed layer factor. Finally, factor 9 was regarded as temperature influenced because of warm species *G. menardii tumida* and *G. menardii flexuosa* relationship (Hemleben et al., 1989). When taken factor scores into account along with biostratigraphic zones Y and Z and oxygen isotopic data (Figure 8) thermocline (factor 1) seems to go along with the oxygen trend. Thermocline factor behaviour followed the temperate water conditions (factor 2) in the course of biozone Y. The factor interpreted as stratification or salinity variation (factor 3) presented an opposite tendency to factor 4 (linked to *Globigerinella digitata* and *Hastigerina digitata*). From base-core to about 20,000 years ago (biozone Y) mixed layer control (factor 5) seems to mirror factor 6 (*Turborotalia quinqueloba* and *Globoturborotalita tenella*), from then on, the two curves appeared coincident. There were not comparative patterns observed among the other factors.

5. Conclusion

the application of Q- and R-mode factor analysis to microfossil compositional data sets was useful to reconstruct the most prominent environmental parameters inherent to planktonic foraminifera or calcareous nannofossils fluctuations in the past. Greater correlation coefficients (0.9 to average) confers more reliability to the Q-mode technique compared to the R-mode for which only a third of the correlation coefficients were higher than 0.3.

Additionally, the amount of R-mode statistically significant factors was larger. This is consistent with natural conditions where several parameters act simultaneously in a given community. However, interpretations of these factors could be a hard task since factors correlate to species whose ecological preferences are unclear or unknown. A reduced amount of retained factors of Q-mode show a relationship with the most abundant species, yielding easier interpretation parameters.

Comparing the application of both techniques on calcareous nannofossils and planktonic foraminifera it was possible to recognize some similarities among factors. The significance of PC-01 factor 1 and SAN-76 factor 2 Q-mode results are analogous and related to the same time interval: glacial period influenced by surface water productivity. Along these lines PC-01 factor 2 (nutricline/thermocline) and SAN-76 factor 1 (mixed layer) indicates the control of water stratification during the interglacial.

Temperature-related R-mode factors (PC-01 factor 1; SAN-76 factor 2 and 9) attend to the same biota response although any temporal connection could be found. In this way PC-01 factor 2 and SAN-76 factor 1 and 5 linked to water stratification. These factors showed oscillating curves throughout the cores, but could be associated to major relevance in biozone Y. Finally PC-01 factor 4 and SAN-76 factor 3 should be considered indicating equivalent conditions since they dwell on productivity inductions (lower vertical gradient) or salinity issues for both groups of organisms.

The lack of correspondence between Q-mode retained factor and those from R-mode approach

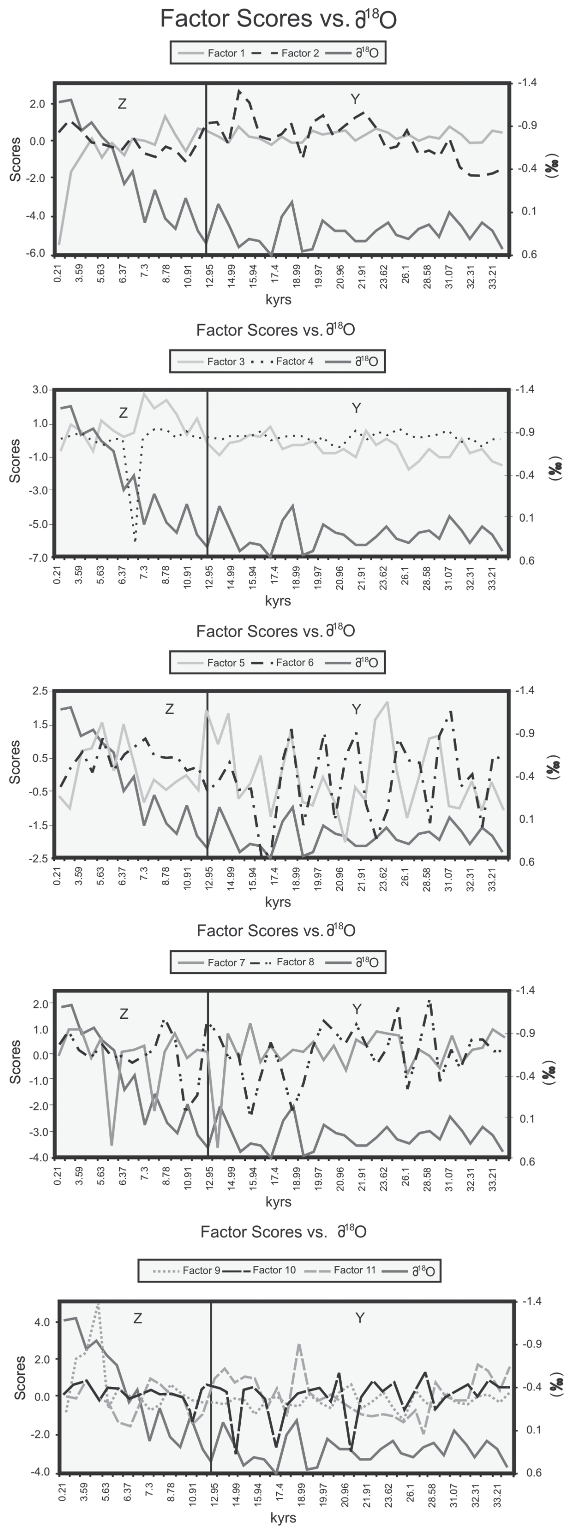


Figure 8 – SAN-76 R-mode factors 1 to 11 scores, oxygen isotopic curve and planktonic foraminifera determined zones Z (interglacial) and Y (glacial)

can be explained by their different function. Once interested in along time samples inter-relationships Q-mode technique should be chosen, however, if species inter-relationship is enquired, then R-mode would be more appropriate.

We believe that as long as we are interested in improving paleoceanographic inferences based on marine micropaleontological quantitative data sets, Q-mode factor analysis is recommended. Q-mode temporal elucidation, its higher reliability regarding correlation coefficients and its finest interpretable results are some advantages pointed out over the R-mode technique.

The complete data set from statistical analysis are available at: http://lapas-io.blogspot.com/2010/10/tabelas-do-artigo-hirama-et-al-2010.html

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