Heavy mineral distributions in offshore sediments using Q-mode factor analysis



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ABSTRACT

Q-mode factor analysis was used on six data sets to evaluate the spatial relationship of offshore sediments via heavy mineral compositions in areas of the Chesapeake Bay mouth and Virginia Continental Shelf. The investigations involved up to 36 minerals and 538 samples. Ilmenite, garnet, pyrobole (amphibole + pyroxene), and to some extent magnetite commonly define factors and end-member sample compositions. For both a small and large number of samples, sediments in the area around Smith Island Shoals and a few other remote locations are mineralogically different from other sampled areas. For most of the investigations, samples fell into offshore or inshore groups, and the inshore group might be further divided into subgroups approximately north and south of the Bay mouth. Mixing is common in the Bay mouth area and several inshore areas.

INTRODUCTION

Heavy minerals in sediment samples obtained from Virginia's coastal regions can be characterized in a number of ways. Here we use modal mineralogy data providing the percent composition of heavy mineral assemblages in the sediments. The relative abundances of a fixed number m of these minerals treated as variables measured on a collection of n sample objects yields an $n \ge m$ data matrix whose structure can be evaluated using eigenvector methods (Davis, 2002). One such method, Q-mode factor analysis, has demonstrated the ability to identify compositional end-members within the data (Klovan and Miesch, 1975; Miesch, 1976; Joreskog and others, 1976; Boon and others, 2018). These end-members (Q-mode factors) can in many cases be regarded as hypothetical or otherwise unknown sample objects whose compositions are mutually independent (uncorrelated with those of any other factor). Perhaps most importantly, the end-members can often be regarded as unique 'source' objects (sediment sources in this case) for comparison with individual samples being evaluated as mixtures of sources.

Q-mode factor analysis of heavy mineral compositions has been used to evaluate the spatial relationship of offshore sediments in areas of the Chesapeake Bay mouth (Berquist, 1986) and Virginia Continental Shelf (Calliari and others, 1990). Both studies show similar results for sediment sources (land and offshore) with complex transport pathways in and out of the Bay mouth region. These interpretations are based on factor (mineral) gradients defined by isopleth maps of sample 'loadings' on each of three factors as explained in the following section.

Q-mode Methods and Terminology

In Q-mode analysis, the term **loading** refers to the projection of a sample vector into factor axis space. Given a set of variables for each sample, such as the abundances of specified minerals reported as a percent of the total, the data are normalized to produce a sample vector of unit length so that the projected loading value ranges from -1 to +1 on the chosen factor axes, as illustrated in Figure 1. As the value of the loading approaches +1 for a given factor, there is a higher degree of compositional similarity between the variables.

The unit circle depicted in Figure 1 represents a cross-section of a three-dimensional sphere upon which the loading values are projected. Note that while only two factor axes are labelled in Figure 1, other factor axes may exist, including one that is normal to the page. In an analysis using three factors, samples that plot close to the origin have a higher loading on factor 3, compared with factors 1 and 2. Still more factors could be added but not visualized in a single drawing. In practice, the analyst specifies a fixed number of factors (usually two, three, or four) needed to explain the variation in the data after which axis rotation is performed that maximizes the spread of projected values on each axis.

The factors themselves are unit vectors located in *m*-dimensional variable space so that their compositions mirror that of the sample objects. However, due to data normalization, a similar set of projected values termed factor **scores** must be used in place of percentages to represent the mineral compositions.



Figure 1. Plot of sample objects in a three-factor solution shown using a two-dimensional factor diagram.

By way of example, Figure 1 depicts the projection of sample 17, which has the observed mineral composition shown in Table 1. Sample 17 has the highest loading on factor 1 of all samples, equal to 0.9771. Figure 2 graphically illustrates the close similarity between the factor 1 scores for each variable and the observed mineral composition of sample 17.

Table 1. Observed percent heavy mineral composition of sample 17.

Sample 17												
variable #	1	2	3	4	5	6	7	8	9	10	11	12
mineral name	ilmenite	rutile	leucoxene	magnetite	monazite	kyanite	zircon	garnet	pyrobole	staurolite	epidote	titanite
% composition	2.73%	0.23%	1.48%	11.96%	0.00%	0.80%	6.61%	4.33%	50.34%	1.82%	16.29%	3.42%



Figure 2. Comparison of the normalized factor scores for each variable (left), and the percent mineral composition of sample 17 (right).

Referring to Figures 1 and 2, the high loading of sample 17 on factor 1 implies a similar, but not identical, mineral composition compared with other samples in the factor 1 space. Q-mode factor analysts weigh the advantages of choosing a small number of factors to evaluate similarity between samples against the loss in communality as indicated by sample vectors that never quite touch the unit sphere for a three-factor solution (see Figure 1). The analytical computations require that all factor axes be mutually orthogonal, which occasionally results in negative scores. It is nevertheless apparent in the above example that sample object 17, and by inference the compositional end-member designated as factor 1, are both enriched in variables 4 (magnetite), 9 (pyrobole) and 11 (epidote) in similar proportions. That the composition of factor 1 is interpreted to represent a hypothetical sediment "source" implies that sample 17 is in the approximate location of that source of sediment material.

Six different investigations were completed in this study using sample data from three main sources herein referred to as ActLabs, Berquist (1990), and Luepke (1990). The ActLabs data source includes analytical data for samples collected as part of a Cooperative Agreement (M14AC00013) between the U.S. Bureau of Ocean Energy Management (BOEM) and the Virginia Department of Mines, Minerals and Energy – Division of Geology and Mineral Resources (DGMR). A full description of the samples and laboratory results reported by Activation Laboratories, Ltd. (Actlabs) is given in Berquist and others (2016), and Lassetter and Blanchette (2019).

Data computations and visualizations were performed using MathWorks MATLAB software. Data files, programs, supporting graphs, tables and other information used in this report are available from the corresponding authors, or by contacting DGMR.

10 MINERALS, 21 SAMPLES

Our initial investigation focused on a relatively small number of core and grab samples collected in 2017 as part of BOEM Cooperative Agreement M14AC00013. Actlabs report A18-05577 contained modal abundances for 36 heavy minerals in 21 sediment samples that were collected in four main areas offshore of Virginia's coast. We chose 10 titanium (Ti)-bearing minerals (Table 2) for the matrix of 10 variables x 21 samples, and the compositions were normalized to sum to 100%. The lab results reported for the mineral "ilmenite" were not used in this analysis because its abundance in most of the samples, averaging 32 weight percent of the total heavy mineral fraction, was so much greater than any of the other Ti-bearing minerals that it would have overshadowed the variance and analytical potential of the other minerals.

ID	mineral
1	ilmenite lower Ti
2	pseudobrookite
3	rutile
4	rutile-altered (leucoxene)
5	pseudorutile
6	leucoxene
7	ilmenite-silicate mixed
8	rutile-qz texture
9	hematite-Ti
10	titanite

Table 2. Ti minerals, less ilmenite, and their ID numbers used in the 10 x 21 data matrix.

Figure 3 shows the 21 samples plotted in two-dimensional factor space and that there are two distinct groups of minerals based upon how the samples load onto defined factor 1 and factor 2. Five samples from the Actlabs report (sample IDs 10, 11, 12, 13, and 14) are more closely associated with factor 2 than the remaining samples that load more highly on the factor 1 axis. The mineral composition of factor 1 is shown in Figure 4, and consists mostly of "rutile" and "rutile-altered". The composition of factor 2 is shown in Figure 5 and implies nearly even abundances of most of the Ti minerals in the Actlabs report.



Figure 3. Two-dimensional plot of a two factor solution for 21 samples, 10 Ti-bearing minerals (unit circle not shown).



Figure 4. Rutile and rutile-altered (ID 3 and 4) are predominant in the composition of factor 1.



Figure 5. The composition of factor 2 has nearly equivalent relative abundances of most of the Ti minerals.

A plot of the geographic locations of the 21 samples shows four of the five samples most closely associated with factor 2 (sample IDs 11, 12, 13, and 14) located in the area of the morphologically distinct feature, Smith Island Shoals (Figure 6). The fifth sample that also loaded highly on factor 2 (sample ID 10) is located far to the north of the shoal area. This suggests that the sediment compositions in the shoal location and the location of sample 10 have a nearly even abundance of all Ti minerals (factor 2), and that the average abundances of rutile and rutile-altered minerals are less than those in the other samples. The remaining 16 samples that loaded highly on factor 1 show no obvious association with a distinct morphological feature on the continental shelf based on this analysis.

The goals of this initial investigation of a small number of minerals (variables) and samples were to gain some preliminary insight into the factor analysis data matrix, the compositional relationships of samples to one another, to see if there was separation of samples into different groups, and if so, what variables or minerals defined the groups. Although the number of samples was small, the compositional differences between the two identified groups could have several explanations.

Rather than interpreting two different sediment sources with mixing, there may be common factors in the physical conditions of the sea bottom at the locations of sample 10 and Smith Island Shoals samples. Based on heavy mineral compositions, sediments in the region of Smith Island Shoals and sample 10 might be derived from an older (pre-Holocene?) source area such as a partially preserved barrier island complex. Alternatively, both areas may be subject to a unique current regime with selective sorting of transported minerals. To better understand these

possibilities, Smith Island Shoals might be a target for future studies. It would be very difficult to discover two separate groups of samples by mere inspection of the Actlabs report. We conclude that the compositions of heavy minerals in the shoal area and at the location of sample 10 are distinct, but the underlying reasons for the similarity remain uncertain.



Figure 6. Locations of 21 samples (10 x 21 matrix) from Actlabs report A18-05577.

24 MINERALS, 125 SAMPLES

Previous studies of heavy minerals in the Chesapeake Bay and Inner Continental Shelf of Virginia relied on optical identification techniques. Twelve to fifteen major minerals were identified and were common to all reports. The automated ActLabs procedure produced 36 different minerals; most of these were reported in low abundance and likely would have been optically classified as "other", or included in a commonly identified group such as magnetite. Working toward being able to combine Actlabs and previous data, we reduced the number of Actlabs minerals by adding minerals reported in low abundance to respective major mineral groups or excluding them from the analysis (tourmaline, for example). The sample abundances reported by Actlabs for the minerals hematite-Ti, mag/hema, goethite, boehmite, chromite, chromite with low Al-Mg magnetite were added to the abundance of magnetite. The minerals ilmenite-lower Ti and ilmenite-silicate mixed were added to ilmenite. Finally, pseudobrookite, rutile, rutile-altered (lower Ti), pseudorutile and rutile-qz texture were added to rutile. Combining minerals this way mimics the process used in earlier studies to optically estimate mineral abundances. Thus, a data matrix of 24 minerals and 125 samples was created.

For this study, we used a three factor solution. In Figure 7, the samples appear to plot in at least two main groups, one as a band of points farthest from the origin in this two-dimensional diagram, which represent "mixtures" of factors 1 and 2, and the other near the origin, loading high on factor 3 (and possibly additional factors), which is perpendicular to the Figure. Another way to view results of the three factor solution is shown in Figure 8.



Figure 7. Two-dimensional plot of a three factor solution for 125 samples, 24 minerals.



Figure 8. Three-dimensional plot of a three factor solution for 125 samples, 24 minerals.

Within the MATLAB program, Figure 8 may be rotated for three-dimensional viewing. Most all of the samples plot on the shell of a sphere in the positive quadrants for all three factors. The red-colored dots are the three samples (numbered 18, 90, and 124) that are closest in composition to the scores of each of the three independent factors. There is no obvious grouping of samples in factor space similar to Figure 3 but rather a continuum across the quadrant's sphere. The composition of sample 18 closely approximates the scores of factor 1 and is enriched in garnet. The composition of sample 124 closely approximates the scores of factor 2, rich in amphibole abundance. Sample 90 associates most highly with factor 3 defined by abundant ilmenite.

To understand how samples relate to one another and facilitate geologic interpretations of the data, samples may be plotted on a chart and factor loadings contoured to define gradients and possible sediment transport pathways and directions. This procedure was applied by Berquist (1986) and Calliari and others (1990). Because samples for this study are spread across the offshore region of Virginia in a narrow band that is only several miles wide, we chose to classify the loadings and plot them on a chart using ArcMap 10.4 software.

Loadings on factor 1 were divided into three classes (classified) in ArcMap and plotted on a chart, Figure 9. This map plot suggests that there are two groups of minerals, one offshore enriched in garnet and one close to shore with mixing at the Bay mouth.



Figure 9. Map of classified loadings on factor 1 (garnet), 125 samples x 24 minerals.



Figure 10. Map of classified loadings on factor 2 (amphibole), 125 samples x 24 minerals.

The distribution of samples loading highly on factor 2 (amphibole) appear mostly inshore with some mixing offshore as shown in Figure 10. Ilmenite-enriched factor 3 samples are distributed across the study area with local mixing (plot not shown). Overall, these plots show two groups of sediments, inshore and offshore.

Several non-heavy minerals were reported in the Actlabs analyses, and the group of 24 minerals shows some contribution of quartz, carbonates, feldspar, etc. All samples were subjected to a sink-float process in a heavy liquid to eliminate minerals having a specific gravity of less than 2.96. However, composite grains composed of two or more minerals (quartz and ilmenite for example) were included in the sink fraction and explains why minerals of low specific gravity were included in the Actlabs analyses. We chose to eliminate reported abundances of non-heavy minerals and create a new data set of only 19 minerals and 125 samples.

19 MINERALS, 125 SAMPLES

The minerals used in this analysis are listed in Table 3. A four factor solution was chosen and the mineral scores (compositions) for each factor are shown in Figures 11, 12, 13 and 14.

ID	mineral
1	ilmenite
2	rutile
3	leucoxene
4	magnetite
5	spinel
6	monazite
7	xenotime
8	florencite
9	apatite
10	kyanite
11	zircon
12	garnet
13	pyroxene
14	amphibole
15	mica
16	staurolite
17	wollastonite
18	schorl-tourmaline
19	epidote

Table 3. Minerals and their ID numbers used in the 19 x 125 data matrix.



Figure 11. Mineral composition (scores) of factor 1 includes mostly garnet, also ilmenite, magnetite, and staurolite (ID numbers 1, 4, 12, 16).



Figure 12. Mineral composition (scores) of factor 2 include mostly amphibole.



Figure 13. Mineral composition (scores) of factor 3 include mostly ilmenite.



Figure 14. Mineral composition (scores) of factor 4 include mostly magnetite.





The map plot of loadings on factor 1 (Figure 15) again shows two groups of minerals, inshore and offshore, with mixing in the Bay mouth area, similar to the investigation of the 24x125 data (Figure 9). However, a map plot of sample ID numbers and loadings on factor 4

shows samples at the Smith Island Shoals area (and sample 98) distinct from the rest of the offshore based on their magnetite abundance, similar to Figure 3 and Figure 6. Three other samples in this data (4, 33, and 69) load heavily on factor 4. If at some future date the significance of minerals at Smith Island Shoals is determined, one might apply that to the locations of these other remotely located samples.



Figure 16. Map of classified loadings on factor 4 (magnetite), 125 samples x 19 minerals, also showing sample ID numbers.

ECONOMIC MINERALS: 10 MINERALS, 125 SAMPLES

DGMR provided a list of heavy minerals with economic interest. Those minerals are listed with their ID in Table 4 and are the basis for a 10x125 data matrix. A three factor solution was run and Figure 17 shows sample loadings plotted in factor 1 and factor 2 space. In this investigation, samples 87, 88, and 89 appear as outliers, but load heavily on factor 3 (Figure 18) in factor 2 and factor 3 space. Factor 1 is composed mostly of ilmenite (Figure 19) whereas factor 2 is composed of a relatively even abundance of nearly all the economic minerals (Figure 20). Factor 3 is defined by abundant kyanite.

ID	mineral
1	ilmenite
2	rutile
3	leucoxene
4	titanite
5	monazite
6	xenotime
7	florencite
8	apatite
9	kyanite
10	zircon

Table 4. Minerals and their ID numbers used in the 10 x 125 data matrix.



Figure 17. Two-dimensional plot of a three factor solution for 125 samples, 10 economic minerals.



Figure 18. Two-dimensional plot (factor 2 -factor 3 space) of a three factor solution for 125 samples, 10 economic minerals.



Figure 19. Mineral composition (scores) for factor 1 include mostly ilmenite.



Figure 20. Mineral composition (scores) for factor 2 are relatively equivalent for most of the economic minerals.

Figure 21 shows the locations of samples for this analysis with the classified loadings on factor 1 (ilmenite). This plot shows nearly all the offshore samples are characterized by a relative abundance of ilmenite. From the 10x125 data matrix, ilmenite is the most abundant heavy mineral with an average of 60% and standard deviation of 11.8% (within the normalized group of economic minerals). The map distribution of samples loading high on factor 2 occurs in the Bay mouth area (Figure 22) where sediment mixing is common. There, almost all of the economic minerals have a relatively even abundance.

Figure 21. Map of classified loadings on factor 1 (ilmenite), 125 samples x 10 economic minerals.

Figure 22. Map of classified loadings on factor 2 (similar mineral abundances of nearly all the economic minerals), 125 samples x 10 economic minerals.

Factor 3 is composed mostly of kyanite (Figure 23). The three outlier samples are located east of the Bay mouth where they alone show highest loadings on factor 3 (Figure 24). It is not clear why only these three samples are prominent. There are places on the Inner Shelf where pre-Holocene strata are exposed, and it might be that the heavy mineral compositions of those

sediments differ from younger sediments. If so, perhaps these samples are located in older sediments exposed on the sea floor.

Figure 23. Mineral composition (scores) for factor 3 show kyanite is the predominant heavy mineral.

Figure 24. Map of classified loadings on factor 3 (kyanite), 125 samples x 10 economic minerals.

12 MINERALS, 538 SAMPLES

We wanted to use Q-mode factor analysis to investigate as much of the available offshore heavy mineral data as possible, but encountered several problems. First, the data sources do not report abundances for the same suite of heavy minerals; for example, whereas Actlabs reported individual percent abundances for amphibole and pyroxene, Berquist (1990) reported combined abundances of these two minerals designated as "pyrobole". Second, ilmenite abundances reported by Luepke (1990) were consistently lower by about 25% when compared to the Actlabs and Berquist (1990) data. Lastly, the interpretation of our factor analysis results relies upon map plots of the factor loadings. Samples from core sections below the surface section were considered important to include, but confounded two-dimensional map plots because numerous samples were "stacked" at the same geographic location.

Nevertheless, samples from Luepke (1990) and Berquist (1990) were added to the Actlabs data for a combined total of 538 samples. Twelve minerals were common to these studies and are listed in Table 5. The original abundances of these minerals were normalized for each data set before combining. A four factor solution was chosen and the factor scores are shown in Figures 25 through 28. The significance of this investigation is identifying the minerals that define the different factors and end-member samples in this large data set. They are "pyrobole" (combined pyroxene and amphibole), ilmenite, garnet, and to a lesser extent magnetite, garnet and epidote. Factor loading map plots are shown in Figures 29 through 32 for this investigation.

ID	mineral
1	ilmenite
2	rutile
3	leucoxene
4	magnetite
5	monazite
6	kyanite
7	zircon
8	garnet
9	pyrobole
10	staurolite
11	epidote
12	titanite

Table 5.	Minerals	and	their ID	numbers	used	in	the	12	х :	538
and the	12 x 304 o	data 1	matrix.							

Figure 25. Mineral composition (scores) for factor 1 show the predominant heavy mineral to be pyrobole (pyroxene + amphibole).

Figure 26. Mineral composition (scores) for factor 2 show the predominant heavy mineral is ilmenite.

Figure 27. Mineral composition (scores) for factor 3 show the predominant heavy mineral is garnet.

Figure 28. Mineral composition (scores) for factor 4 shows the predominance of magnetite, with some garnet and epidote.

Figure 29. Map of classified loadings on factor 1 (pyrobole), 538 samples x 12 minerals.

Figure 30. Map of classified loadings on factor 2 (ilmenite), 538 samples x 12 minerals.

Figure 31. Map of classified loadings on factor 3 (garnet), 538 samples x 12 minerals.

Figure 32. Map of classified loadings on factor 4 (magnetite), 538 samples x 12 minerals.

Figures 29 through 32 show there are groups of minerals associated for the offshore, inshore, Bay mouth and north, and Bay mouth and south. Mixing is common in the Bay mouth and in several places inshore. This data set includes all core sections, surface and at depth, and it is unknown which core section shows on these plots.

12 MINERALS, 304 SAMPLES

For this investigation, we used data from Actlabs reports and Berquist (1990) and the same 12 minerals presented in Table 5. However, we eliminated samples from core sections below the surface core section. This step provided minerals data that most likely represents only Holocene-age sediments in the offshore and Bay mouth areas. The core samples are considered to be compatible with seafloor grab samples because they probably exclude late Pleistocene (or pre-Holocene) strata.

A three factor solution was used and the distribution of samples in three-dimensional factor space is shown in Figure 33. Most of the 304 samples plot in the positive factor 1, 2, and 3 quadrants. Samples 30, 124 and 289 are shown in red and are the end-members most closely aligned with factors 1, 2, and 3, respectively.

Figure 33. Three-dimensional plot of a three factor solution for 304 samples, 12 minerals.

The scores for factor 1 and the observed mineral composition of sample 30 are shown in Figure 34. Note the overall similarity to each other, particularly for garnet and pyrobole (Table 5, mineral IDs 8 and 9). The scores for factor 2 and composition of the end-member sample 124 are shown in Figure 35 and rely heavily on the abundance of ilmenite (Table 5, mineral ID 1). The scores for factor 3 and the composition of the end-member sample 289 (not shown graphically) indicate a predominance of pyrobole with lesser ilmenite.

Figure 34. Comparison of the normalized factor 1 scores for each variable (left), and the percent mineral composition of sample 30 (right).

Figure 35. Comparison of the normalized factor 2 scores for each variable (left), and the percent mineral composition of sample 124 (right).

The classified loadings on factor 1 are displayed in Figure 36, which shows the endmember sample 30 is located far offshore in the designated Virginia Wind Energy Area. This plot shows the predominance of garnet and pyrobole in the offshore sediments, with mixing from other sources in the Bay mouth and Eastern Shore areas. Figure 37 shows that factor 2 ilmeniterich samples represent inshore areas, with mixing across the study area. Figure 38 is a map plot of factor 3 classified loadings, showing an abundance of pyrobole-ilmenite sediments inshore and south of the Bay mouth. End member sample 289 is located at the Smith Island Shoals area. Overall, the analysis suggests two groups of sediments, one inshore and one offshore.

Figure 36. Map of classified loadings on factor 1 (garnet and pyrobole), 304 samples x 12 minerals.

Figure 37. Map of classified loadings on factor 2 (ilmenite), 304 samples x 12 minerals.

Figure 38. Map of classified loadings on factor 3 (pyrobole and ilmenite), 304 samples x 12 minerals.

SUMMARY AND CONCLUSIONS

The outcome of subjecting mineral compositions of a large number samples to factor analysis was meant to gain some insight into the data matrix and to display the relationship of samples to one another. Because most of the samples are located close to shore and are not distributed across the Inner Shelf, sediment sources and transport pathways are difficult to define. However, the spatial clustering of samples with similar mineral compositions is evident in the results. Using Q-mode factor analysis, this report shows several results. First, several minerals commonly define factors and end-member sample compositions. They are ilmenite, garnet, pyrobole, and to some extent magnetite. Second, for both a small and large number of samples, sediments in the area around Smith Island Shoals and a few other remote locations are mineralogically different from other sampled areas; these areas might be targeted for future work. Third, for most of the investigations, samples fall into offshore or inshore groups. The inshore group might be divided into subgroups approximately north and south of the Bay mouth. Mixing is common in the Bay mouth area and several inshore areas.

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