Classification of rock types using multivariate analysis in the Dezak area, SW Iran

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Abstract

The geochemical multivariate techniques were applied to recognize different geological units and categorized rock types which accompanied by different penalties. Knowing changes and classification of raw materials with macroscopic and microscopic quantification have direct effect on economic and efficiency in a precipitated calcium carbonate plant. Based on lithological changes, the Dariyan Formation was divided into four rock units based on a total of 492 chip samples collected from the study area. The main aim objective of this study was to classify the rock types in this area using a multivariate analysis combining the R-mode factor analysis and K-Means method. Due to the opposite vector orientation of SiO_2 , Al_2O_3 , Fe_2O_3 , K_2O , MgO , Na_2O , MnO , TiO_2 , P_2O_5 , SrO , and SO_3 versus CaCO_3 , the lowest geochemical similarity and maximum separation distance were observed between CaCO_3 and other parameters using the R-mode factor analysis, which has also been verified by the Ward's hierarchical agglomerative clustering method. Complementary Q-mode analysis was applied to determine the position of the samples (eigenvalues) with respect to the variables (eigenvectors). In order to geochemical classification of the samples, the K-Means clustering method classified the samples taken from the study area into four geochemical groups. The second group, which comprised a total of 422 composite samples, contained high-concentration CaCO_3 samples with an average concentration greater than 97%. The average SiO_2 concentration in these samples was 1%, and the sum of Al_2O_3 and Fe_2O_3 was about 0.38%. Therefore, the materials falling in this group can be appropriately used as raw materials to feed the plant. Using clr-transformed data for R- and Q-mode analysis, the eigenvectors and eigenvalues show sub-compositionally coherent and closure effect is overcomes. The total variance which is explained by the first factor decreases from 78.6% in real R-mode analysis to 61.7% in clr transformation. Due to major occurrence of the first dimension on geochemical changes, the samples categorized as richest (the best data set), contaminated (the worst data set), and transmission zone.

Keywords Dariyan Formation · R-mode factor analysis · K-Means clustering · Precipitated calcium carbonate (PCC) · Micritic and crystallized limestone · Clr transformation

1 Introduction

Although the limestone formation is widely extended across Iran, not many areas are available from which precipitated calcium carbonate (PCC) can be industrially produced. The PCC is the most important product produced

from limestone mineral processing [41]. This product is used in a variety of industries including pharmaceuticals, paper industries, and cosmetics [23]. Papers made from CaCO_3 have a low production cost and high quality and offer advantages such as environment-friendly properties, reduced water consumption, higher printing resolutions,

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increased resistance, waterproof properties, and resistance to oil and insects [26]. Therefore, the PCC industry plays an important role in the paper production across the world. To prepare PCC, high-purity limestone reserves must be available in large amounts. Moreover, the extracted materials should have a minimum amount of penalty elements such as silicic components and Fe_2O_3 , and suitable infrastructure and conditions should be provided for the mining processes [25].

The Dezak limestone area is located at 30 km south-east of Shahrekord, in Chahmahal-va-bakhtiari provinces, SW Iran [14]. The Dariyan Formation in the High Zagros zone is strongly covered by shallow limestone with wackestone–packstone textures preserved from the lower Cretaceous. It is composed of medium-bedded gray limestone. The lower and upper boundaries gradually transition to the Fahliyan and Kazdomi Formations, respectively. This area is a potential site for industrial survey project of PCC. A systematic sampling was designed in order to identify the properties of the rock units. The results from XRF analysis were interpreted by the multivariate and univariate analyses. Due to the compositional specification of the variables and existence of penalties, the selection of the CaCO_3 -richest materials is not the only goal. Based on compositional properties of the data in geochemical processes, the samples and variables must be interpreted simultaneously. Therefore, multivariate analysis would be applied in order to identification of CaCO_3 -rich zone with a minimum amount of penalty elements. Accordingly, R-mode and Q-mode analysis and K-Means methods could help to explore the relationship between elements and samples. Factor analysis (FA) and the cluster and K-Means analyses are the most frequently used multivariate methods in the literature to explore the relationship between elements and samples [21, 22, 34]. These methods are employed to reduce the dimension for variability between data sets [9, 43]. In this manuscript, the clr-transformed data have been used by robust R-mode analysis, while they obtained by the CoDaPack software v 2.01 (available at <http://www.compositionaldata.com/>). The compositional data in geochemical samples reveal the nonnegative value for elements (indicated as vectors in R-mode graphical outcomes) and sum to a constant [38].

From a tectonic point of view and considering the sedimentary facies and structural style in SE Iran, the Darian, Gadvan, and Kazhdumi are the essential formations in the Dezak area, SW Iran [7]. The lower boundary of the Darian Formation gradually fades and reaches the Gadvan Formation, but from above it is strongly eroded with Kazhdumi Formation and separated by the oolitic and glauconite layers [19]. The Dariyan limestone separates the Gadvan (below) and Kazhdumi (above) Formations. This formation is known as a part of the Cretaceous (Lower Cretace)

sequence in the southwest of Iran [32]. Darian is the most important reservoir in the Zagros basin for hydrocarbon accumulations southwest of Iran [27]. The Shaiba Formation south of Persian Gulf can be considered a similar formation located in the countries in this region [30, 37]. The Darian Formation includes about 286.5-m-thick brown–gray limestone abundant with orbitalina [33].

The first major goal of the study was the identification and classification rock types in the Dezak area based on the geochemical data and using a multivariate analysis combining the R-mode analysis and K-Means methods. The geological evidence and specimen properties must be consistent in the geochemical analysis. To this end, a CaCO_3 -rich zone with a minimum amount of penalty elements must be identified, for which the following steps should be taken: (1) exploration of the best lithologies that cover the main concepts, (2) identification of distinct rock units both geologically and geochemically, and (3) area classification based on the amount of the main components so as to provide an appropriate feed zoning.

2 Geological setting

The exploration operations around the village of Dezak in Chaharmahal and Bakhtiari Province began in late 2016 to identify and supply raw materials to the PCC plant. The location map of the Dezak limestone exploration area in structural map of Iran is shown in Fig. 1. Prior to this, the prospecting and exploration phases were completed in an area of 15 km² (1:10,000 scale) along with a semi-detailed exploration in a 2-km² area (south east of the preliminary exploration area). This basic exploration area is depicted by a red polygon. Moreover, the figure shows the two exploration license areas (highlighted in pink) and the area considered for the detailed exploration phase (marked by a yellow polygon covering 150 hectares).

The geological map of Dezak (scale 1:1000) for the detailed exploration phase is depicted in Fig. 2. The map covers an area of 150 hectares. The topography of the area is highly irregular as it is located on the margin of the main Zagros fault zone. The overall lithological sequences contain cretaceous sediments from Darian and Kazhdumi Formations. Based on lithological changes, the Darian and Kazhdumi Formations were divided into 4 and 1 units, respectively.

Thick-bedded to massive light gray to gray recrystallized and micrite limestone with intercalations of thin-bedded orbitalina limestone contains orbitalina and bivalves fossils and is indicated by K_d^I unit. Thick- to medium-bedded light gray to gray limestone with intercalations of thin-bedded marl was introduced as K_d^{Im} . The boundary of the K_d^I and K_d^{Im} units on the west side of the

contains bivalves and orbitolina fossils and is denoted by K_d^{ml} . Thick- to medium-bedded gray to light gray limestone fossiliferous bivalves include chert nodulose

Fig. 3 **a** Boundary of the limestone and the marl with interbedded limestone unit on the west of the detailed exploration area, **b** a view of the limestone layers in the center of the area, **c**, **d** different

views of the limestone layers on the east of the area, **e** a view of the iron oxide veins inside the limestone layers, **f** a view of the orbitolina fossils found within the limestone layers

and are presented by K_d^{II} unit. Alternation of thin-bedded dark gray silty shale and marl with intercalations of thin-bedded limestone contains bivalves and ammonite fossils, which are associated with the Kazhdumi Formation, and is indicated by K_{KZ}^{sh-m} . Gravel fan and young terraces (Q_t) and recent alluvium and river beds (Q_{tl}) are the other recent sediments (Fig. 2). Iron oxide veins in slight amounts have been observed inside the limestone layers (Fig. 3e). Orbitolina fossils found within the limestone layers in K_d^I and K_d^{II} units are depicted in Fig. 3f.

3 Materials and methods

3.1 Sampling and stratigraphic column

Systematic sampling was carried out for carbonate rocks and other units using a regular grid of 40 m × 40 m. Multiple chip samples were collected from each square box, and all samples were packed as a composite sample (Fig. 4). Each box corresponding to a laboratory sample, a total of 492 samples (originated from 2024 chip sample) were collected from the area. Due to the impossibility of sampling, some of the considered samples were not

Fig. 4 Systematic sampling of area in the exploration phase. The profile of Seghalat (name of the valley) is schematically

Table 1 Classified types for the field samples in the exploration phase

Sample type	Total samples	Final composite samples
Crystallized and micritic limestone samples	1890	421
Marl samples	98	62
Limestone and marl (mixed sample)	28	7
Chert–limestone	8	2

extracted during the sampling operation. Finally, a total of 421 samples were taken from the crystallized and micritic limestone, 62 samples from the marl unit, 7 samples from the limestone and marl (mixed sample) units, and 2 samples from the chert–limestone rocks (Table 1). All samples were subjected to X-ray fluorescence analysis (XRF) to measure their major oxides.

Moreover, the Seghalat profile was designed to plot a stratigraphic column over the area. The position of this profile is shown in Fig. 4. Overall, eight samples were taken from 10KLED063 to 10KLED070, each composed of several subsamples (Fig. 5). The actual thickness of the stratigraphic unit (m) varied from 10 to 60 m (as minimum and maximum, respectively), with a total thickness of roughly 177 m (Fig. 6). Important notes regarding each lithology in this stratigraphic column are given in Fig. 6.

3.2 Compositional data analysis

Regarding the statistical methods, there are several normalization schemes for compositional data that should probably be applied here prior to any clustering or factor analysis. According to specification of geochemical data and their spatial distribution, the closure effect is not avoided for real data. In order to avoid the closure effect of element, the data should be opened using log-ratio transformation [6, 10, 15, 17, 28]. The clr, the ilr, and alr transformation are the different type of log-ratio transformation [5, 8, 36, 44]. The alr and clr transformations were already defined by Aitchison [5]. One example normalization technique is the centered log-ratio (clr) method, but there are several others (isometric log-ratio is another). Methods, applications, and calculation software for these normalization schemes are readily available for free online (e.g., CoDaPack).

3.3 Hierarchical clustering and R-mode analysis

A dendrogram (hierarchical clustering) is capable of decomposing data objects into several levels of nested partitioning (as a tree of clusters). Clustering of the data objects is carried out by cutting the dendrogram at the desired level, where each connected component forms a cluster. Ward's method is a variance-based method derived from agglomerative hierarchical clustering [29]. Variance methods generate clusters to minimize the intra-cluster variance [11, 40, 42]. For each cluster, the sum of

Fig. 5 **a** An image of sample 10 K-LED063 at its location, **b** sampling location of 10 K-LED065, **c** image of starting point of sample 10 K-LED066, **d** overview of the location for sample 10 K-LED068, **e**

overview of the location for samples 10 K-LED069 and 10 K-LED068, **f** image of sampling end point for Sample 10 K-LED070 in Seghalat profile

squares is calculated, and the two clusters with the smallest increase in the overall sum of squares within cluster distances are combined. Ward's method and the average linkage method have been shown to perform better than the other procedures [35, 39].

Clustering is the classification of objects into different groups, or more precisely, the partitioning of a data set into subsets (clusters), so that the data in each

subset could share some common similarity according to some defined distance measure [3, 4, 12, 31]. Factor analysis takes as input a large number of variables and describes them with small number of factors in order to reduce the data dimension [1, 2, 18, 20]. Appropriate factors should provide an easy interpretation of the data to make geological sense. In addition, simple presentation of anomalies, elemental association, and represent

Fig. 6 Stratigraphical column with rock units in the Seghalat profile

indicative samples are the other benefits of the multi-variate method.

3.4 K-Means clustering

The k-means method is an algorithm that clusters n given objects into k partitions based on their attributes, where $k < n$. It is similar to the expectation-maximization algorithm for mixtures of Gaussians in that they both attempt to find the centers of natural clusters in the data [13, 24].

K-Means algorithm is useful for undirected knowledge discovery and is relatively simple. K-Means has found widespread usage in many fields such as unsupervised learning of neural network, classification analysis, pattern recognitions, image processing, machine vision, and artificial intelligence [16]. Each cluster is represented by the center of the cluster, and the algorithm converges

to stable centriods of clusters. The most commonly used measure of similarity is the Euclidean distance.

4 Discussion and results

4.1 Statistical parameter

A number of statistical concepts such as mean, standard deviation, variance, minimum, first quartile, median, third quartile, and maximum of the most important elements are given in Table 2. It can be seen that the total mean of CaCO_3 is close to 93% and its standard deviation is 11.795. In addition, 25% (first quartile) of the CaCO_3 data are lower than 95.93%, and 25% more than 97.657%. The variations of CaCO_3 concentration with respect to standard deviation are depicted in Fig. 7, showing changes between < -2.8 SD

Table 2 Statistical properties of the data set in the Dezak area

Variable	Mean	SD	Variance	Minimum	Q1	Median	Q3	Maximum
CaCO ₃	92.958	11.795	139.125	36.209	95.931	97.178	97.657	98.771
SiO ₂	3.501	7.085	50.194	0.08	0.68	0.98	1.78	43.26
Al ₂ O ₃	0.9052	1.896	3.595	0.01	0.16	0.25	0.41	9.42
Fe ₂ O ₃	0.3702	0.763	0.5822	0.03	0.09	0.12	0.17	4.82
Na ₂ O	0.03596	0.04557	0.00208	0.01	0.02	0.02	0.03	0.36
K ₂ O	0.165	0.2867	0.0822	0.01	0.04	0.06	0.1175	1.85
MgO	0.7477	0.4271	0.1824	0.31	0.51	0.595	0.78	3.42
TiO ₂	0.04756	0.08429	0.0071	0.008	0.017	0.02	0.025	0.536
MnO	0.02099	0.017729	0.000314	0.014	0.015	0.016	0.017	0.24

Fig. 7 Changes in CaCO₃ concentration based on standard deviation

and 0.25–0.48 SD. Therefore, left-skewness (with a left tail thicker than that of a normal distribution) is identified by negative values for CaCO₃.

The lowest CaCO₃ concentration is 36.209% (Table 2). Since the average CaCO₃ concentration is 93% and the mean concentration is 97.65%, most data are in the positive range of the average value (Fig. 8). Kriging estimation of CaCO₃ based on fractal distribution of data is shown in Fig. 8. Few data are in a range lower than $\bar{x} - 2.8s$, and most have values greater than $\bar{x} - 0.25s$.

Furthermore, the variations in the concentration of SiO₂ are plotted based on half of the standard deviation

(Fig. 9), where the kriging estimation was carried out with a search radius of 50 m. Due to the sensitivity and effects of penalties on the high-grade CaO zone, the estimations were carried by using just one sample from each side. The average concentration of SiO₂ falls in the first range of standard deviation ($\bar{x} \pm 0.25s$), and with gradual changes up to $\bar{x} + 2.7s$, the concentration increases from 0.18 to 37.41% (Fig. 9). The gradual concentration changes in Fe₂O₃, Al₂O₃, MgO, K₂O, and Na₂O are shown in the ranges of 0.03–4.82, 0.02–9.25, 0.31–2.55, 0.01–1.85, and 0.01–0.33% of the variations, respectively.

Fig. 8 Kriging estimation of CaCO_3 based on fractal distribution of data

Fig. 9 SiO_2 concentration changes based on standard deviation

4.2 Geochemical multivariate analysis

4.2.1 Hierarchical clustering and factor analysis

Clustering and factor analysis were performed on all the 492 samples obtained from a systematic grid sampling. Ward's agglomerative clustering starts with CaCO_3 and LOI in a separate cluster for the Dezak samples. On the other hand, $(\text{SiO}_2, \text{Al}_2\text{O}_3)-(\text{Fe}_2\text{O}_3, \text{TiO}_2)-\text{K}_2\text{O}$ are formed and linked to MnO due to maximum similarity. Na_2O , MgO and P_2O_5 are then added to them to increase the cluster sizes. All the mentioned components connected to SO_3 according to having the smallest similarity. Eventually, the components $(\text{SiO}_2, \text{Al}_2\text{O}_3)-(\text{Fe}_2\text{O}_3, \text{TiO}_2)-\text{K}_2\text{O}$, MnO, Na_2O , MgO, P_2O_5 , and SO_3 were classified in the same cluster, such that its distance is maximum from CaCO_3 (or equally, the similarity is a minimum value) (Fig. 10).

Using factor analysis, it was shown that the CaCO_3 and LOI characteristics have the highest similarity and the most geochemical proximity (Fig. 11a). Due to the opposite eigenvectors (loading) of SiO_2 , Al_2O_3 , Fe_2O_3 , K_2O , MgO, Na_2O , MnO, TiO_2 , P_2O_5 , SrO, and SO_3 versus CaCO_3 , the lowest geochemical similarity and maximum separation distance between CaCO_3 and other parameters were observed (Fig. 11a). Hence, with a decrease in CaCO_3 , the other parameters are more likely to increase. The intensity and weight of changes in the investigated characteristics or eigenvectors (R-mode analysis, Fig. 11a) can be fully investigated by another analysis that will determine the position of the samples revealed by eigenvalues (Q-mode analysis, Fig. 12a).

4.2.2 K-Means analysis

By incorporating the results of multivariate K-Means analysis into the graphical Q-mode factor analysis, the variability of the data could be categorized as four geochemical data sets (Fig. 13). The geochemical classification is based on the results of K-Means multivariate analysis. Based on the eigenvectors of the data in Fig. 11a and K-Means classification in Fig. 13, the second group shows a CaCO_3 enrichment of above 97%, while the first group indicates intermediate grades below 50% (Fig. 14). The first geochemical group comprises 21 samples and contains the highest concentration of SiO_2 with an average greater than 30% (Table 3). The second group, which comprises 422 composite samples from the region, also contain high-concentration CaCO_3 samples with an average value greater than 97% (Table 3). The average SiO_2 concentration in these samples is 1%, and the sum of Al_2O_3 and Fe_2O_3 is about 0.38% (Table 3). The second group has the lowest mean distance from the center (Fig. 13) as well as the highest CaCO_3 concentration (97%). It is observed that most of the samples are indicative of CaCO_3 concentration and some samples show depletion. Sample Nos. S436 and S445 have the least CaCO_3 concentration (Fig. 13). On the other hand, a limited number of samples (S150, S56, and S410) show the highest SO_3 concentration in the area.

4.2.3 Clr-transformed data analysis

In the present manuscript, the authors have used the robust factor analysis (RFA), and RFA based on clr

Fig. 10 Ward linkage and correlation coefficient distance for Dezak samples

Fig. 11 Eigenvectors of geochemical parameters for normal scores data indicate 87% of variation (**a**) and clr-transformed data indicate 70% of variation (**b**) at Dezak area

transformation in order to better elemental evaluation in Dezak area. By comparison of the results from R-mode on real data and R-mode on clr-transformed data, the closure effect is overcome. Where real data are opened by R-mode analysis, the eigenvectors maybe overlaid; while using compositional data transformed by log-ratio transformation, the eigenvectors show inherence. Log-ratio transformation analysis is sub-compositionally coherent so in this respect is better. This is because compositional data sum to 100% (closure), which explains why, e.g., CaO and LOIs are on opposite sides of PC1 from SiO₂, etc. The

R-mode analysis opened by real data is shown in Fig. 11a, and it shows sub-compositional incoherence. For this normal score or the real data, the majority of the variations (78.6%) are enclosed to first factor and all the vectors are separated in the semicircle.

By using clr-transformed data for R-mode analysis, the eigenvalues show sub-compositionally coherent and closure effect is overcome. Accordingly, the total variance which is explained by the first factor decreases from 78.6% in real R-mode analysis to 61.7% in clr transformation (Fig. 11a, b). This indicates the highest effect of

Fig. 12 Eigenvectors of geochemical parameters and eigenvalues of 492 samples on the PC1 versus PC2 for normal scores data indicate 87% of variations **(a)** and clr-transformed data indicate 70% of variations **(b)** at Dezak area

CaCO_3 parameter for the first factor in the robust method (Fig. 11b). The results after transformation in R-mode analysis are mostly constrained and represented in a full circle.

Besides, the incoherence between scores of samples (Fig. 12a) was overcome by clr transformation in Q-mode analysis (Fig. 12b). Finally, clr-transformed data indicate two population in Q-mode graphical representation, which is separated by distinct anisotropic clouds (Fig. 12b). Due to major occurrence of the first dimension, the geochemical changes are categorized as richest

(the best data set), contaminated (the worst data set), and transmission zone (Fig. 15). The linkages between them are well explained as:

The best data set = the richest rock units of limestone include K_d^1 and K_d^{lm}

The transmission zone = Marginal data or the CaCO_3 unit with marl and Shale

The worst data set = the light gray marl include K_d^{ml} .

Fig. 13 Q-mode of factor analysis accompanied by K-Means clustering

Fig. 14 Overlay clustering of the geological map using geochemical analysis. Code 2 with a CaCO_3 concentration of higher than 97% is considered an appropriate population

Interval plot of CaCO_3 for groups obtained from multivariate K-Means analysis represents the mean value, and the mean value plus and minus the standard deviation ($x = \bar{x} \pm s$), as shown in Fig. 16. The mean values observed

in each group are the same as those previously calculated in Table 2 using the K-Means method. As seen, Cluster 2 shows the highest CaCO_3 concentration (97.02%; Fig. 16). The standard deviation of CaCO_3 concentration in the second

Table 3 Average concentration of variables in each cluster obtained from K-Means analysis

Variable	Cluster 1	Cluster 2	Cluster 3	Cluster 4
CaCO ₃	48.0977	97.0268	66.9833	86.1376
SiO ₂	30.3624	1.0568	18.7948	7.9554
Al ₂ O ₃	8.0571	0.2558	5.1374	1.9262
Fe ₂ O ₃	3.346	0.1221	1.8635	0.6731
Na ₂ O	0.1795	0.0236	0.09	0.0727
K ₂ O	1.2357	0.072	0.7374	0.3031
MgO	1.9919	0.6503	1.38	0.765
TiO ₂	0.3756	0.0202	0.2124	0.0805
MnO	0.0851	0.0164	0.0445	0.0234
P ₂ O ₅	0.112	0.0344	0.0877	0.0613
SO ₃	0.03	0.0214	0.0282	0.0549
LOI (1000)	27.0507	43.149	33.9036	39.6584
LOI (1100)	27.2405	43.4084	34.0952	39.8542

set of the data is 0.10 with a confidence level of 95% (CI %). The values are calculated as follows:

$$x = \bar{x} - s = 97.02 - 0.10 = 96.92$$

$$x = \bar{x} + s = 97.02 + 0.10 = 97.12.$$

If the analyzed data have been investigated on the basis of field observations, based on the geochemical properties of the samples, these changes will show up according to the following groups in the area:

- The first group contains crystallized and micritic limestone (with numerous FeX and Cal veins and veinlets): This group with average CaCO₃ and SiO₂ concentrations of 30% and 48%, respectively, belongs to the marl rocks. The highest amount of Al₂O₃ and Fe₂O₃ is also observed in this group, while the MgO content is about 2%. This group is illustrated in Fig. 14 with a red circle. These samples have high overlap with the K_d^{ml} unit and represent marl samples. This layer is the transitional zone (code 1) and in field observation detected as marl or limestone and marl (mixed sample) samples.
- The second group contains about 50% micritic limestone and 50% alluvial limestone, < 50% limestone, and probably chert–limestone: This group is illustrated in Fig. 14 with a black circle. These samples are highly uniform and have an overlap with the K_d^{lm} and K_d^l units. It can be seen that there exists an undesirable discrepancy between the 95% CI obtained from the 2th group and the other three groups (Fig. 16). This group belongs to the high-quality limestone group in the area with

Fig. 15 Scores plot on the PC1 versus PC2 for clr-transformed data accompanied by categorized samples at Dezak area. Due to major occurrence of the first dimension, the geochemical changes cate-

gorized as richest (the best data set), contaminated (the worst data set), and transmission zone

Fig. 16 Interval plot of CaCO_3 in five groups obtained from the multivariate K-Means analysis

mean concentrations of 97% and 1% for CaCO_3 and SiO_2 , respectively.

- The third group includes 50% < marl, 50% > debris and limestone (marl sample): With an average concentration of 67% and 19%, respectively, for CaCO_3 and SiO_2 , this group belongs to the intermediate or transition groups. This group is illustrated in Fig. 14 with a yellow symbol. These samples clearly indicate the boundaries of K_d^{lm} , K_d^{l} , and K_d^{ml} units or a mixture of them.
- The fourth group consist of 1) 50% < crystallized limestone and micritic rocks and 50% > marl and debris; 2) about 50% chert–limestone and about 50% marl and debris (mixed sample). The fourth geochemical group with an average concentration of 86% and nearly 8%, respectively, for CaCO_3 and SiO_2 belongs to the poor quality limestone group of the region. This group is illustrated in Fig. 14 with a red symbol. Samples in this group are also located at the border, but are more inclined toward the K_d^{l} and K_d^{lm} units.

The spatial plot of the samples in the area is depicted in Fig. 14. The second group (represented with Code 2) mainly consists of K_d^{lm} and K_d^{l} lithologies. They were covered by thick- to medium-bedded light gray to gray limestone and thick-bedded massive light gray recrystallized and micrite limestone containing orbitalina and bivalves' fossils, respectively. Accordingly, comprehensive information can be obtained from the spatial position of the samples and lithologies. The first and third groups are relatively CaCO_3 -depleted samples. Therefore, each geochemical group that represents a certain concentration

of its compounds is directly linked to a geological code. Thick- to medium-bedded gray (or light gray) limestone and thick-bedded light gray recrystallized and micrite limestone containing orbitalina and bivalve fossils.

5 Conclusion

This study concluded that the second group can be considered as the best plant feed from both spatial and geochemical perspectives. With a CaCO_3 concentration of higher than 97% and SiO_2 concentration lower than 1%, this group was recognized as the high-quality limestone group in the area. These samples are highly uniform and overlap with K_d^{lm} and K_d^{l} units, so thick-bedded gray (or light gray) agglomerated units of micritic and recrystallized limestone are the main important lithologies. This layer contains thin layers of orbitalina limestone containing orbitalina fossils. On the other hand, the K_d^{ml} unit revealed that marl layer is the transitional zone and is the most inappropriate feed layer. Due to the high overlap between the classified samples and the geological map, both of them are verified by remarkable note in package samples and visual properties; all the classifications have been confirmed. Moreover, geochemical analyses confirmed the geological properties in the area, such that K_d^{lm} and K_d^{l} rock types from light gray to gray colors contained micritic and crystallized limestone as the most important units.

In order to overcome closure effect at the area, compositional clr transformation was done. Accordingly,

semicircular eigenvector (loadings of elements) and eigenvalues (score plot of samples) in normal distribution could be seen in a circular and anisotropic distribution by clr transformation. Scores plot on the PC1 versus PC2 for clr-transformed data accompanied by categorized samples at Dezak area. Due to major occurrence of the first dimension, the geochemical changes categorized as richest (the best data set), contaminated (the worst data set), and transmission zone.

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Compliance with ethical standards

Conflict of interest The authors have no affiliations with or involvement in any organization or entity with any financial interest, or non-financial interest in the subject matter or materials discussed in this manuscript.

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