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e-ISSN: 2774-2016 - https://journal.itera.ac.id/index.php/indojam/
p-ISSN: 2774-2067

K-Means Clustering to Enhance the Petrified Wood Composition Data Analyses and Its Interpretation

Received 24th March 2023
Accepted 8th June 2023
Published 31st July 2023

Open Access

DOI:
10.35472/indojam.v3i1.1288

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Abstract: Geologically, the fossilization of wood materials into fossils requires appropriate conditions, some of which have been preserved for millions of years. In nature, the organic mass of wood must be quickly replaced by inorganic elements before it decomposes under harsh geological conditions. Anorganic oxides such as silica-oxide, are known to be the main components of most wood specimens (up to 80%). The presence of alkaline oxides such as sodium and potassium oxide seems to play a major role in the presence of dissolved silica during petrification. However, their significance in the petrification phenomenon that occurs in fossilized plant wood is not yet known. Therefore, in this study, cluster analysis was conducted to determine the relationship between the presence of silica and alkaline compounds in petrified wood fossils. The approach used was ***k***-means clustering supported by the Silhouette Coefficient Method, which aims to review and order a complex set of data into subsets, thus allowing interpretation. The results showed that the clustering of the fossil wood composition data was optimal at ***k*** = 3. There is a fair correlation between the presence of silica and alkali oxide compounds (-0.504 to -0.387), as well as with another inorganic compounds (+0.957). The presence of sodium and potassium is strongly correlated during silicification (+0.905). Additionally, the results of data clustering made the wood fossilization process susceptible to describe, especially through data regression. The data visualization provides more facts and proper explanations of the role of alkaline oxides in wood silicification. This study furthers our understanding of wood fossilization, especially the diagenesis of wood chemical composition in geological history.

Keywords: *k-means clustering, silhouette coefficient method, data regression, fossil, wood petrification*

Abstrak: Proses perubahan kayu menjadi fosil membutuhkan kondisi dan waktu yang benar-benar tepat. Materi-materi organik harus segera tergantikan oleh unsur anorganik sebelum terdekomposisi oleh kondisi alam. Elemen seperti silika diketahui menjadi komposisi utama pada kebanyakan spesimen kayu yang ditemukan (>80%). Keberadaan unsur alkali seperti natrium dan kalium nampaknya memiliki peranan besar dalam hadirnya silika terlarut dalam proses petrifikasi. Hanya saja belum diketahui signifikansinya dalam fenomena petrifikasi yang terjadi pada fosil tumbuhan berbahan kayu. Untuk itu dalam studi ini dilakukan analisis korelasi untuk mengetahui kaitan antara kehadiran silika dan senyawa alkali pada fosil kayu yang telah tersilifikasi. Pendekatan yang dilakukan adalah melalui ***k***-Means Clustering yang ditunjang dengan Silhouette Coefficient Method, yang bertujuan untuk mereview dan membagi sekumpulan data komplek menjadi subset, sehingga lebih mudah diinterpretasi. Hasil menunjukan bahwa pengelompokan data fosil kayu optimal pada ***k*** = 3. Terdapat korelasi antara kehadiran silika denan senyawa alkali oxide (-0,504 to -0,387), serta senyawa anorganik lainnya (+0.957). Keberadaan natrium dan kalium memiliki korelasi kuat saat silisifikasi berlangsung (+0.905). Selain itu hasil clustering data membuat proses fosilisasi kayu menjadi lebih mudah dideskripsikan melalui hasil regresi data yang dihasilkan. Pada hasil visualisasi data tersebut, memberikan gambaran yang lebih deskriptif tentang pernanan senyawa alkali pada peningkatan kehadiran silika oksida pada petrifikasi kayu. Studi ini dapat membawa pemahaman yang lebih mendalam pengenai proses fosilisasi kayu, terutama pada proses perubahan komposisi kimia yang terjadi sepanjang sejarah geologi.

Kata Kunci: *k-means clustering, metode silhouette coefficient, regresi data, fosil, petrifikasi kayu*

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Introduction

Geological records have shown that wood fossils are majorly found that already naturally silicified. These fossils are millions of years old and are still well-preserved, even on the cellular scale [1-3]. It has already replaced carbon-based organic wood fiber with various anorganic oxides, such as silica, manganese, iron, and copper. Seemly, it infiltrated by the rich-soluble mineral, which was suspended in the mud-fluid during fossilization and petrified after [4,5]. It changes the wood material into a solid anorganic material, which forms an array of colors that vary greatly. For example, quartz crystals have no color, but when contaminants are added during the petrification and /or weathering process, the crystals will have fascinated shades of yellow, red, or other colors, depending on their chemical composition [5-7].

Wood fossils can be differentiated by hardness, luster, preserved wood fibers, and various colors, all of which are influenced by the chemical composition of the fossil [3,4]. The age of wood fossils greatly influences the maturity of mineralization owing to harsh geological conditions (some take millions of years). Wood fossils can be found in various sizes ranging from log forms to fragments. However, wood fossil 'maturity' can be distinguished by their density and mineral composition. This is because the mineral structure changes and forms gradually and continuously, replacing the bio-organic structure of wood [1,5]. Recently, the process of chemical changes in wood fossils has been investigated. Some researchers have suspected that the silification process plays a major role. However, the presence of silica must be supported by alkaline pH conditions and the appropriate temperature. A more quantitative examination of the gradient of chemical composition changes in wood fossil is required. In this study, we approached this through clustering analysis.

Clustering is the process of dividing a set of data objects into subsets, called clusters. Objects in a cluster have properties that are similar to each other and different from those of other clusters [8,9]. Clustering is the grouping of data based on the similarity of the characteristics of each part of the data. In this research, the K-means method was used, along with optimizing the determination of the number of clusters using the silhouette coefficient method.

K-Means clustering is a non-hierarchical clustering method that seeks to partition existing objects into one or more groups, where objects with similar characteristics are grouped into the same cluster, and objects with different characteristics are grouped into other clusters [10-12]. In addition, k-means clustering also groups data based on the distance between the data and cluster centroid point obtained using an iterative process. To choose number k as the input of the algorithm, an analysis needs to be performed. The purpose of k-means clustering is to obtain data groups by maximizing the similarity of features within clusters and the differences between clusters [13-16].

Different numbers of clusters from the same dataset yield different evaluation values. The selection of the silhouette coefficient method is used to generate information to determine the optimal number of clusters by looking at the quality of the clusters and how well an object is placed in a cluster. The results of the different silhouette coefficients for each cluster value can be seen using a graph [14,15].

From this research, it is expected that correlation analysis and clustering results using the k-means method and optimization of the number of clusters using the silhouette coefficient method will produce optimal clusters and provide useful information regarding wood fossils based on their geochemical composition.

Method

A. Correlation.

The correlation is an indicator of the strength of the linear relationship between two variabels, namely x and y [10], where, r is the correlation coefficient, see Equations (1).

$$r = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sqrt{n\sum_{i=1}^{n} {x_i}^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\sqrt{n\sum_{i=1}^{n} {y_i}^2 - \left(\sum_{i=1}^{n} y_i\right)^2}} \quad (1)$$

B. Silhouette Coefficient.

The silhouette coefficient method combines cohesion and separation measures for cluster evaluation [12]. Calculating the cohesion involves measuring the distances between all objects within a cluster, while measuring the separation involves determining the distances between each object and its nearest neighboring cluster. The steps for computing the silhouette coefficient are as follows:

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1. Calculate the average distance of a data point, denoted as i, to all other data points within the same cluster using Equation (2).

$$a(i) = \frac{1}{|A| - 1} \sum_{A, j \neq i} d(i, j) \quad (2)$$

2. where j represents other data points within the same cluster A, and $d(i, j)$ represents the distance between data point i and j.
3. Calculate the average distance of the data point i to all data points in other clusters and take the minimum value using Equation (3).

$$d(i, c) = \frac{1}{|A|} \sum_{j \in c} d(i, j) \quad (3)$$

where $d(i, c)$ represents the average distance of data point i with all data points in cluster c, where $A \neq c$.

$$b(i) = \min_{A \neq c} d(i, c) \quad (4)$$

4. Calculate the Silhouette Coefficient value using Equation (5):

$$s(i) = \frac{b(i) - a(i)}{\max\big(a(i), b(i)\big)} \quad (5)$$

The silhouette coefficient method is used to fine the optimal number of clusters. The selection of the best k (number of clusters) value is based on the highest silhouette coefficient value [12].

The changes in the value of k and silhouette coefficient value are presented in the form of xy line-graphs.

C. *k*-Means Clustering

The k-means clustering algorithm is a non-hierarchical clustering method that minimizes within-cluster variance and maximizes the variance between different clusters [13]. The k-means clustering algorithm consists of the following steps**:** choose k (random) data points to be the initial centroid (cluster centers) [14]. Assign each data point to the closest centroid and use Equation (6).

$$\mu_i = \frac{1}{N} \sum_{i=1}^{N} x_i \quad (6)$$

Re-compute the centroid using the current cluster memberships using the Euclidean Distance [9], as shown in Equation (7),

$$D(x_i, \mu_i) = \sqrt{\sum_{k=1}^{p} (x_{ik} - \mu_{ik})^2} \quad (7)$$

If a convergence criterion is not met, the steps in Equations (6) and (7) are repeated. If the cluster center no longer changes (converges to single value), then the clustering process is complete.

This process was performed using Google Colabolatory [17] (Python programming language facility from Google).

Result and Discussion

Dataset

The dataset of the composition of wood fossils consists of 93 compiled data points with four chemical variables related to wood fossils [18], which are the geochemical compositions of wood fossils, namely SiO_2, K_2O, Na_2O, dan other compositions, pada **Table 1**.

Table 1. Compilation of the geochemical composition of wood fossils

ID	Sample	w (%)			
		SiO_2	K_2O	Na_2O	Others
1	1-BHK-1/1	90.254	0.063	0.059	8.857
2	1-BHK-1/2	92.954	0.045	0.012	6.544
3	1-BHK-1/3	91.053	0.022	0.028	8.040
4	2-BHK-2b/1	93.505	0.033	0.036	6.247
5	2-BHK-2b/2	93.357	0.038	0.030	6.203
6	2-BHK-2b/3	93.117	0.027	0.037	6.499
7	3-BHK-2g/1	94.386	0.009	0.010	5.356
8	3-BHK-2g/2	93.509	0.030	0.011	6.145
9	3-BHK-2g/3	94.420	0.027	0.009	5.237
10	4-KDH/1	95.136	0.025	0.029	4.485
11	4-KDH/2	91.387	0.016	0.004	7.914
12	4-KDH/3	95.353	0.017	0.002	4.425
13	5-KDH-1a/1	90.735	0.055	0.017	7.016
14	5-KDH-1a/2	94.119	0.050	0.035	5.372
15	5-KDH-1a/3	88.497	0.069	0.011	10.098
16	6-KDH-2b/1	94.885	0.019	0.002	4.415
17	6-KDH-2b/2	94.808	0.011	0.001	4.452
18	6-KDH-2b/3	95.681	0.012	0.000	3.553
19	7-KDH-2r/1	94.371	0.000	0.000	5.596
20	7-KDH-2r/2	95.131	0.041	0.009	4.792

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ID	Sample	w (%)			
		SiO_2	K_2O	Na_2O	Others
21	7-KDH-2r/3	95.196	0.014	0.011	4.738
22	8-KDH-D10/1	88.700	0.026	0.003	10.837
23	8-KDH-D10/2	89.280	0.028	0.005	10.586
24	8-KDH-D10/3	88.303	0.020	0.000	11.385
25	9-KDH-D1b/1	91.578	0.030	0.009	7.722
26	9-KDH-D1b/2	89.440	0.034	0.016	10.033
27	9-KDH-D1b/3	89.055	0.009	0.000	10.221
28	10-KDH-D1br/1	90.277	0.025	0.038	9.158
29	10-KDH-D1br/2	90.908	0.041	0.001	8.855
30	10-KDH-D1br/3	90.764	0.012	0.026	9.113
31	11-KDH-D2/1	88.263	0.025	0.000	11.589
32	11-KDH-D2/2	88.393	0.008	0.000	11.379
33	11-KDH-D2/3	89.487	0.012	0.004	10.376
34	12-KDH-E1/1	89.871	0.020	0.015	9.882
35	12-KDH-E1/2	88.567	0.023	0.008	11.204
36	12-KDH-E1/3	88.658	0.025	0.000	11.229
37	13-KDH-3W/1	94.941	0.034	0.014	4.857
38	13-KDH-3W/2	95.927	0.040	0.011	3.906
39	13-KDH-3W/3	95.455	0.043	0.006	4.435
40	14-KDH-3r/1	97.378	0.018	0.011	2.220
41	14-KDH-3r/2	98.015	0.021	0.000	1.708
42	14-KDH-3r/3	96.215	0.026	0.020	3.528
43	15-KDH-K1o/1	89.857	0.049	0.000	9.843
44	15-KDH-K1o/2	90.199	0.040	0.000	9.437
45	15-KDH-K1o/3	90.822	0.119	0.081	8.794
46	16-KDH-K1w/1	89.166	0.029	0.008	10.646
47	16-KDH-K1w/2	91.480	0.051	0.012	7.901
48	16-KDH-K1w/3	89.839	0.018	0.000	10.082
49	17-KDH-K1b-w/1	89.099	0.049	0.003	10.757
50	17-KDH-K1b-w/2	89.239	0.070	0.047	10.618
51	17-KDH-K1b-w/3	88.916	0.084	0.010	10.810
52	18-KDH-Oo/1	88.674	0.125	0.361	10.693
53	18-KDH-Oo/2	82.051	0.575	5.093	11.163
54	18-KDH-Oo/3	90.834	0.050	0.271	8.403
55	19-KDH-Oy/1	88.041	0.124	0.036	7.533
56	19-KDH-Oy/2	87.006	0.142	0.372	9.278
57	19-KDH-Oy/3	88.643	0.142	0.015	8.408
58	20-KDH-Or/1	82.729	0.218	0.777	15.070
59	20-KDH-Or/2	96.559	0.019	0.006	3.152
60	20-KDH-Or/3	95.958	0.030	0.039	3.765
61	21-CYP-A1/1	96.414	0.016	0.004	3.469
62	21-CYP-A1/2	94.629	0.025	0.045	4.782
63	21-CYP-A1/3	94.620	0.040	0.043	4.962
64	22-CYP-A6/1	92.370	0.045	0.041	7.057
65	22-CYP-A6/2	94.809	0.057	0.036	4.769
66	22-CYP-A6/3	94.504	0.039	0.057	5.120
67	23-CYP-1(NSG-1)/1	88.928	0.100	0.060	9.818
68	23-CYP-1(NSG-1)/2	85.511	0.067	0.050	13.482
69	23-CYP-1(NSG-1)/3	96.852	0.038	0.037	3.022
70	24-TAK-1/1	95.830	0.048	0.043	3.868
71	24-TAK-1/2	93.550	0.043	0.033	6.115
72	24-TAK-1/3	95.920	0.045	0.001	3.825
73	25-TAK-2/1	95.639	0.061	0.023	3.763
74	25-TAK-2/2	95.103	0.025	0.018	4.357
75	25-TAK-2/3	91.456	0.078	0.032	4.032
76	26-TAK-3c/1	96.823	0.003	0.017	3.059
77	26-TAK-3c/2	95.477	0.027	0.003	4.411
78	26-TAK-3c/3	96.556	0.029	0.000	3.363
79	27-TAK-3g/1	95.947	0.008	0.003	3.985
80	27-TAK-3g/2	96.052	0.029	0.000	3.768
81	27-TAK-3g/3	96.052	0.028	0.022	3.770
82	28-TAK-D1/1	96.273	0.037	0.011	3.566
83	28-TAK-D1/2	95.723	0.059	0.029	3.873
84	28-TAK-D1/3	95.893	0.090	0.007	3.737
85	29-TAK-E1br/1	96.255	0.045	0.029	3.596
86	29-TAK-E1br/2	96.960	0.043	0.000	2.858
87	29-TAK-E1br/3	96.731	0.030	0.000	3.100
88	30-TAK-E1g/1	97.028	0.044	0.007	2.801
89	30-TAK-E1g/2	96.398	0.040	0.000	3.448
90	30-TAK-E1g/3	97.254	0.029	0.000	2.629
91	31-TAK-F1/1	95.689	0.091	0.012	3.916
92	31-TAK-F1/2	95.120	0.069	0.018	4.496
93	31-TAK-F1/3	94.903	0.100	0.017	4.635

Data analyses results

Correlation matrices were constructed to examine the characteristics of the level and direction of the

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relationship between the geochemical compositions of each wood fossil. The interval between the correlation values ranged from 0 to 1. The closer the correlation value is to 1, the stronger is the level of relationship between the variables; the closer the correlation value is to 0, the weaker is the level of relationship between the variables. The direction of the relationship between each geochemical composition can be seen as positive (+) or negative (−). A positive sign (+) indicates that if one variable increases, the other variable also increases, or vice versa. The negative sign (-) indicates that if one variable decreases, the other increases, and vice versa. From the data in Table 1, a correlation analysis was carried out using Equations (1) and (2), and the correlation matrix results are shown in Table 2.

Table 2. Correlation Matrix

	SiO_2	K_2O	Na_2O	Others
SiO_2	1.000	-0.504	-0.387	**-0.957**
K_2O	-0.504	1.000	**0.905**	0.304
Na_2O	-0.387	**0.905**	1.000	0.213
Others	**-0.958**	0.285	0.214	1.000

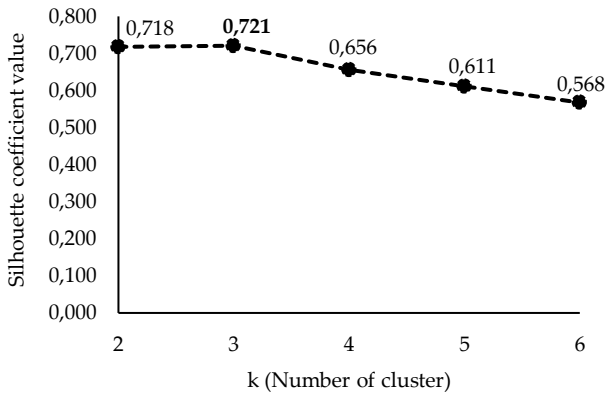

Figure 1. Line graphs of *k*-value (number of cluster) and silhouette coefficient value each parameter. The graph shows that the highest silhouette coefficient value point is 0.721, which was determined as the selected cluster number chosen in this study.

From Table 2, it is known that the level of relationship between the K_2O compound and Na_2O is very strong (0.905), and the direction of the relationship is positive (+), where if the K_2O value increases, the Na_2O value will also increase, and vice versa. The level of relationship between the SiO_2 compound and other compounds is also very strong, with the direction of the relationship marked as negative (-), which means that if SiO_2 increases, then other compounds decrease, and vice versa. This indicated that fossil wood is closely related to SiO_2, K_2O, and Na_2O.

Furthermore, the silhouette coefficient method was used to determine the appropriate optimal k for k-means clustering. The silhouette coefficient value was obtained visually, as shown in Figure 1. In Figure 1, the best or most appropriate and optimal k value is located at the highest silhouette coefficient value point close of 0.721, that is, k = 3, or can be grouped into three.

Subsequently, k-means clustering was applied to the dataset, with k as the centroid of 3. The results of the k-means clustering is shown in Table 3. The results in Table 3 are shown in Figures 2, 3, 4, and 5.

Table 3. Numerical resume of *k*-means clustering result of each parameter

	Data (n)	Min	Max	Std	Centroid
Cluster 1					
SiO_2	53	92.954	98.015	1.152	95.460
K_2O	53	0.000	0.100	0.021	0.035
Na_2O	53	0.000	0.057	0.015	0.016
Cluster 2					
SiO_2	38	85.511	92.370	1.386	89.567
K_2O	38	0.008	0.142	0.038	0.051
Na_2O	38	0.000	0.372	0.090	0.043
Cluster 3					
SiO_2	2	82.051	82.729	0.479	82.390
K_2O	2	0.218	0.575	0.252	0.397
Na_2O	2	0.777	5.093	3.052	2.935

Based on the results of k-means clustering, the geochemical composition of wood fossils is divided into

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three groups: cluster 1 is marked by blue (i.e., a group of wood fossils containing high SiO_2 content), cluster 2 is marked by orange dots (i.e., there are 38 out of 93 data from wood fossils), cluster 3 is marked by yellow dots (i.e., a group of wood fossils containing the highest K_2O and Na_2O), and red dots are centroid points.

The relationship between Na_2O and K_2O in Figure 2 is exponential with the regression model [19,20]:

$$y = 0.0147e^{13.406x} \quad (6)$$

or

$$Na_2O = 0.0147e^{13.406K_2O} \quad (7)$$

The relationship that occurs between SiO_2 and Na_2O in Figure 3 is an exponential relationship with the regression model formed

$$y = 6E + 14e^{-0.405x} \quad (8)$$

or

$$Na_2O = 6E + 14e^{-0.405SiO_2} \quad (9)$$

The relationship that occurs between SiO_2 and K_2O in Figure 4 is a polynomial relationship [13] with the regression model formed:

$$y = -0003x^3 + 0.0957x^2 - 8.8751x + 274.43 \quad (10)$$

or

$$K_2O = -0003SiO_2^3 + 0.0957SiO_2^2 - 8.8751SiO_2 + 274.43 \quad (11)$$

In Figure 4, a confidence interval with 95% confidence interval can be formed using the sample mean and standard deviation, as shown in Figure 5. The confidence intervals measure the level of uncertainty or certainty in the sampling method. Confidence intervals provide more information than point estimates.

Wood silification is a process by which the cell walls of wood are impregnated with silica, leading to the preservation and hardening of the wood. Silica is a naturally occurring mineral that is found in abundance in the environment, and it can bond with the organic material in wood to create a strong and durable composite material. In nature, wood silification occurs over long periods of time, as fallen trees and other woody debris become buried in sediment and are exposed to mineral-rich groundwater [4,21,22]. As the wood decays, the silica in the groundwater replaces the organic material in the cell walls, creating a fossilized wood material known as petrified wood.

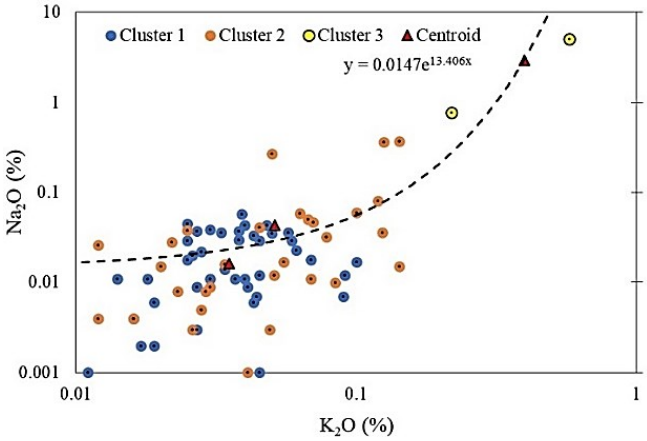

Figure 2. Results of *k*-means clustering and regression line between Na_2O and K_2O

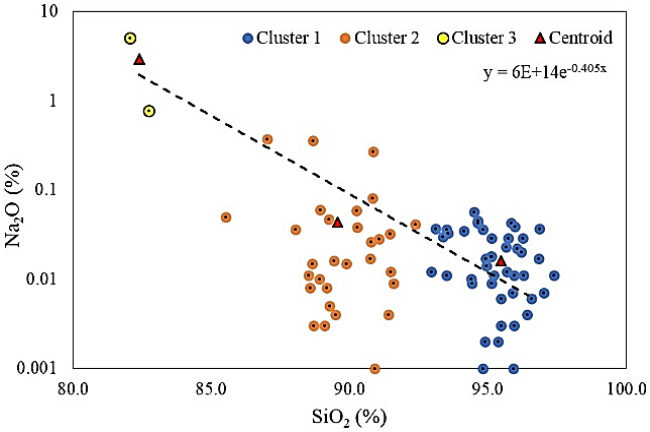

Figure 3. Results of *k*-means clustering and regression line between SiO_2 and Na_2O

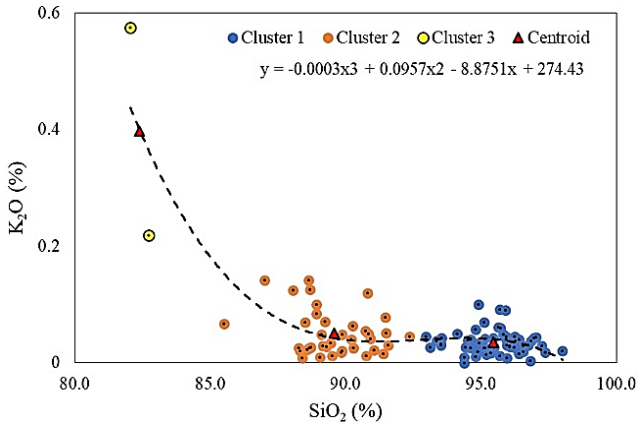

Figure 4. Results of *k*-means clustering and regression line between SiO_2 and K_2O

Sodium and potassium ions acted as precursors for wood silicification. It is present in alkaline water and facilitates silicic acid transport in the drainage

and groundwater. It forms sodium-potassium silicates. When wood is treated with sodium and potassium silicate, silicate ions react with the wood fibres to create a silica gel within the cell walls [2,3,22]. This gel can then be transformed into a solid silica-rich material via a process called consolidation. Geologically, the silica forms opal, chalcedony, and quartz during diagenesis and mineralization [23,24].

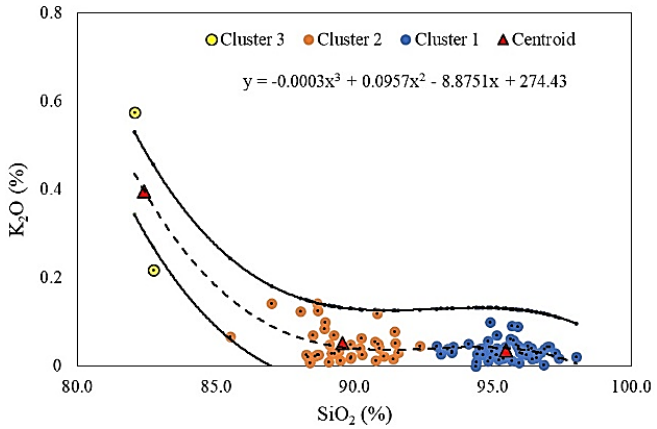

Figure 5. Results of *k*-means clustering, regression line, and confidence interval between SiO_2 and K_2O

Finally, we obtained a better understanding of the chemical compositional changes that occurred. There was a clear degree of silicification in the wood fossilization process based on clustering analysis. When it reached 80%, silica continued to increase, with a subsequent decrease in sodium and potassium. In addition, it can be seen that the presence of sodium is relatively coincident with the presence of potassium. Sodium and potassium appear to provide pathways for silicification in fossil wood. The abundance of sodium and potassium clearly plays a major role in the silicification process. As a follow-up for future research, this study needs to be followed up on a review of other chemical compositions as well as a variety of wood fossil samples with silica values less than 80%.

Conclusion

From the results of the above discussion, it can be concluded that *k* -means clustering can form appropriate cluster members in the geochemical composition data of wood fossils. The resulting information is obtained from the optimal cluster using the silhouette coefficient method with $k = 3$. Analysis of the characteristics of each wood fossil cluster can be performed based on correlation and regression analyses of the geochemical composition. The results of this analysis provide further insight into the wood fossilization process for input in next research.

Conflic interest

No conflict interest are declared.

Acknowledment

The authors are very grateful to the anonymous reviewers for their helpful comments, correction, and suggestions that help improving the presentation and quality of this work.

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Published by: Lembaga Penelitian dan Pengabdian Masyarakat (LPPM)
Institut Teknologi Sumatera, Lampung Selatan, Indonesia

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