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A novel correlation study using pearson and spearman algorithms for mineral component-driven strength analysis of geopolymer

Geopolimerin mineral bileşen odaklı dayanım analizi için pearson ve spearman algoritmaları kullanılarak yapılan bir korelasyon çalışması

Yıldıran Yılmaz[1*], *Talip Çakmak*[2], *Zafer Kurt*[2], *İlker Ustabaş*[2]

[1]Department of Computer Engineering, Faculty of Engineering and Architecture, Recep Tayyip Erdoğan University, Rize, Türkiye.
yildiran.yilmaz@erdogan.edu.tr

[2]Department of Civil Engineering, Faculty of Engineering and Architecture, Recep Tayyip Erdoğan University, Rize, Türkiye.
talip.cakmak@erdogan.edu.tr, zafer.kurt@erdogan.edu.tr, ilker.ustabas@erdogan.edu.tr

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Abstract

This study presents a statistical analysis of the relationship between mineralogical properties and mechanical strength parameters between different constituents. Important properties such as compressive and flexural strength are analyzed on sample materials. Two different correlation methods, namely Pearson Correlation Coefficient and Spearman Correlation Coefficient, were used to evaluate the relationship between mineralogical constituents and strength parameters. The results obtained revealed that some mineral constituents showed a significant positive or negative correlation with mechanical strength properties. In particular, lime (CaO) exhibited an excellent positive linear relationship with compressive strength. Similarly, a strong positive monotonic relationship was found between silica (SiO_2) content and flexural strength. The statistical analyses provide an important tool in understanding the influence of mineral constituents on mechanical strength properties. The results of this study provide a valuable guide to understand the role of mineralogical constituents in construction material selection and structural design.

Keywords: Data mining, Pearson algorithm, Geopolymer, Correlation analysis, Compressive analysis.

Öz

Bu çalışma, farklı bileşenler arasındaki mineralojik özellikler ve mekanik dayanım parametreleri arasındaki ilişkinin istatistiksel bir analizini sunmaktadır. Basınç dayanımı ve eğilme dayanımı gibi önemli dayanım özellikleri örnek malzemeler üzerinde analiz edilmiştir. Mineralojik bileşenler ve mukavemet parametreleri arasındaki ilişkiyi değerlendirmek için Pearson Korelasyon Katsayısı ve Spearman Korelasyon Katsayısı olmak üzere iki farklı korelasyon yöntemi kullanılmıştır. Elde edilen sonuçlar, bazı mineral bileşenlerin mekanik dayanım özellikleri ile anlamlı pozitif veya negatif korelasyon gösterdiğini ortaya koymuştur. Özellikle, kireç (CaO) basınç dayanımı ile mükemmel bir pozitif doğrusal ilişki sergilemiştir. Benzer şekilde, silika (SiO_2) içeriği ile eğilme dayanımı arasında güçlü bir pozitif monotonik ilişki bulunmuştur. İstatistiksel analizler, mineral bileşenlerin mekanik mukavemet özellikleri üzerindeki etkisinin anlaşılmasında önemli bir araç sağlamaktadır. Bu çalışmanın sonuçları, mineralojik bileşenlerin yapı malzemesi seçimi ve yapısal tasarımdaki rolünü anlamak için değerli bir rehber sağlamaktadır.

Anahtar kelimeler: Veri madenciliği, Pearson algoritma, Geopolimer, Korelasyon analiz, Basınç dayanımı.

1 Introduction

Concrete may be the most consumed artificial product in the world and is a composite building material consisting of a combination of different materials [1]. The main reason why concrete is used so much is that in addition to its strength properties, its durability properties are also important parameters in the use of concrete. In addition, its easy formability, easy accessibility, and low cost compared to other building materials also increase its usage. Although concrete has such positive properties, the production of cement, which constitutes concrete raw material, causes significant carbon emissions. Currently, the cement industry is the second largest industry in the world after the steel industry and causes carbon dioxide emissions during the production of cement mortar and concrete [2],[3]. Many natural resources and energy are used during cement production. The amount of energy used constitutes 10% of global energy consumption [4]. In addition to energy consumption, carbon dioxide emissions from cement production constitute 7-9% of total emissions [5]-[8]. In order to reduce the negative impact of cement on global warming, there is a worldwide movement to reduce the energy and emissions used in cement production. For this reason, the need of the construction sector for new alternative building materials to cement is increasing day by day. In order to meet this need, new sustainable cement alternative materials are being developed [9]. The importance of sustainable technologies developed to reduce the use of cement is increasing day by day. A new binder known as geopolymer, which stands out as an alternative to cement, has recently gained importance among researchers. Geopolymers resulting from the activation of pozzolanic binders with alkaline activators are one of the leading alternative materials to cement. As a result of the release of alumina and silicas through solutions with alkali activator properties, geopolymers are formed by establishing strong bonds with other molecules [10]. The type and density of the alkali activator used here is an important parameter. Geopolymers have been accepted as an alternative material to concrete due to their strength and durability properties since the day they were discovered [11]-[14]. In the production of geopolymers, a wide range of waste materials such as fly ash, blast furnace slag, alumino

*Corresponding author/Yazışılan Yazar

silicates such as metakaolin, mineral additives can be used as binders. Waste materials used as binders both prevent the damages they may cause to the environment and provide a solution to the storage problem. It also helps to reduce the consumption of natural resources [15],[16].

Although there are negative criticisms about the use of waste glass powders in geopolymer due to their high amorphous structure and unreactive silica content, waste glass powder can be used in geopolymer when activated with alkaline activators [17]-[22]. In order for its silica content to become reactive, it must be exposed to some heat treatment process. There are significant differences in the mechanical properties of geopolymers with and without heat treatment [23]. In many studies, geopolymers produced using waste glass powder have attracted attention with their durability properties as well as their mechanical properties [18],[20]. Fly ash has been one of the cement additives used in the construction industry for a long time thanks to its properties. In addition to its pozzolanic properties, it is widely used for important reasons such as reducing environmental damage and reducing carbon dioxide emissions by reducing the amount of cement to be used [24],[25]. In addition, low cost, easy accessibility and high activity aluminate and amorphous silicate content make the use of fly ash one step ahead in geopolymer production [26]-[28]. Obsidian is a natural volcanic rock, also known as volcanic glass, which is found in glassy structure in nature. Obsidian is formed as a result of rapid cooling of molten magma in the earth. Its high silica content and amorphous glassy structure indicate that its mechanical properties will be in a good direction [28]. As a result of the studies, it has been shown that obsidian shows high pozzolanic properties and can be used as a pozzolanic material [29],[34].

In this study, binders such as waste glass powder, fly ash and obsidian were used in the construction of geopolymer mortars. When the literature is examined, it is seen that the use of fly ash and waste glass powder in geopolymer construction is common in most of the studies. However, there are almost no studies using obsidian as a binder material. There is no research in the literature that analyses any correlation between the chemical contents of geopolymer mortars obtained from XRF analyses and their compressive and flexural strengths. In order to fill this gap in the literature, Pearson coefficient and Spearman coefficient correlation analyses were performed to determine the relationship and the degree of relationship between the compressive and flexural strengths of the chemical material mixture parameters and chemical contents of geopolymer mortars obtained from 12 different mixtures. With this study, the positive and negative effects of the mixture ratios of geopolymer mortars on the compressive and flexural strengths were examined thoroughly. Consequently, this article makes several significant contributions to the field of sustainable construction materials. It addresses the growing need for sustainable cement alternatives, focusing on geopolymers as a promising binder. The research highlights the importance of waste materials, such as waste glass powder, fly ash, and obsidian, as alternative binders in geopolymers, which not only mitigate environmental concerns but also offer solutions to waste storage issues and reduce natural resource consumption. Despite the widespread use of fly ash and waste glass powder in geopolymers, the study addresses a significant gap in the literature by introducing obsidian as a novel binder material. Furthermore, it conducts correlation analyses between the chemical composition and mechanical properties of geopolymers derived from 12 different materials, employing Pearson and Spearman correlation coefficients, to quantify the relationships between mixture parameters and compressive and flexural strengths. This research provides a comprehensive examination of the effects of mixture ratios on the compressive and flexural strengths of geopolymers, filling a critical knowledge gap in the literature.

2 Materials and methods

This section provides an overview of the materials and mixtures utilized in the study, along with the correlation analysis methods applied. A detailed description of the dataset's components and characteristics used for the analyses is included. Figure 1 outlines the laboratory procedures for preparing geopolymer mortar samples and the steps involved in forming the dataset. Figure 2 illustrates the material and mixture parameters comprising the dataset, the chemical composition derived from the XRF analysis of geopolymer mortar samples, the methods employed for correlation analysis, and the relationship between the dataset parameters and the compressive and flexural strengths determined through the analysis.

2.1 Materials

2.1.1 Glass Waste (GW)

The study's GW, which has an average grain size of 40.789 µm, a surface area measurement of 3910 cm²/g, and a specific gravity measurement of 2.6, is the glass used in the buildings' windows.

2.1.2 Obsidian (OB)

The obsidian stones were extracted from the Cagrankaya area in the Ikizdere district of the Turkish province of Rize. The OB powder has a specific gravity of 2.6, an average dimension of particles of 53.786 µm, and an overall surface area of 4730 cm²/g.

2.1.3 Fly Ash (FA)

Zonguldak Catalagzi Power Plant supplied fly ash, which is industrial waste. Class F fly ash with SiO_2+Al_2O_3+Fe_2O_3 values more than 70% is used as a binder in accordance with ASTM C618 [35], and class V siliceous fly ash is utilized in accordance with BS EN 450 [36]. Fly ash has a specific gravity of 2.06 g/cm³ and a total SiO_2+Al_2O_3+Fe_2O_3 content of 87.815. The typical powder dimension of fly ash is 65.574 µm, and its overall surface area is 0.327 m²/g. Table 1 lists the chemical compositions of the materials utilized as obsidian, waste glass powder, and fly ash as determined by XRF studies.

2.2 Data collection

Dataset consists of two-part geopolymers in which obsidian fly ash and waste glass powder are used as binders. Three 40x40x160 mm geopolymer mortar specimens were produced by activating 12 different mixtures obtained as a result of standard mixing of obsidian, waste glass powder and fly ash in different proportions with 12 M NaOH. The compositions and corresponding parameters of the mixtures are summarized in Table 2.

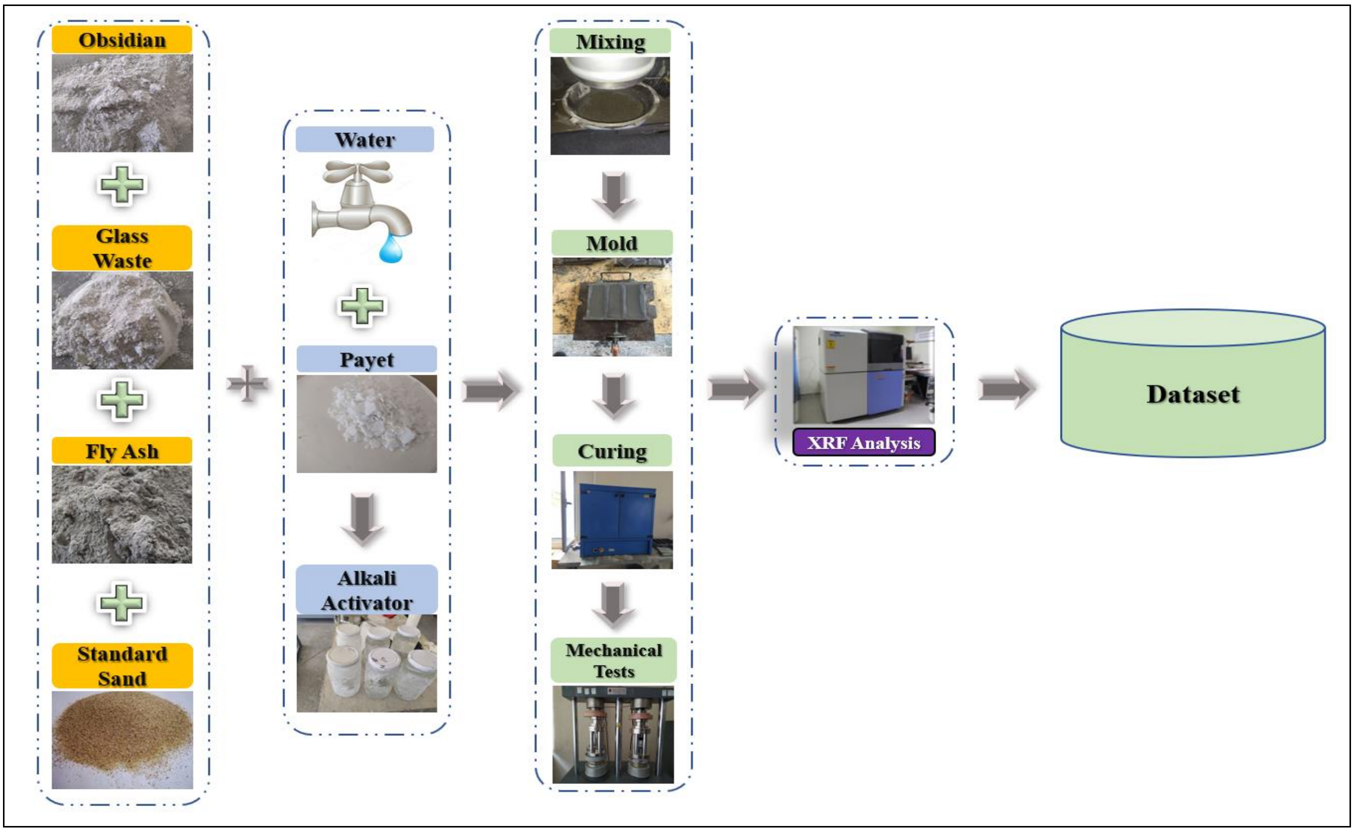

Figure 1. Experiment and data collection scheme.

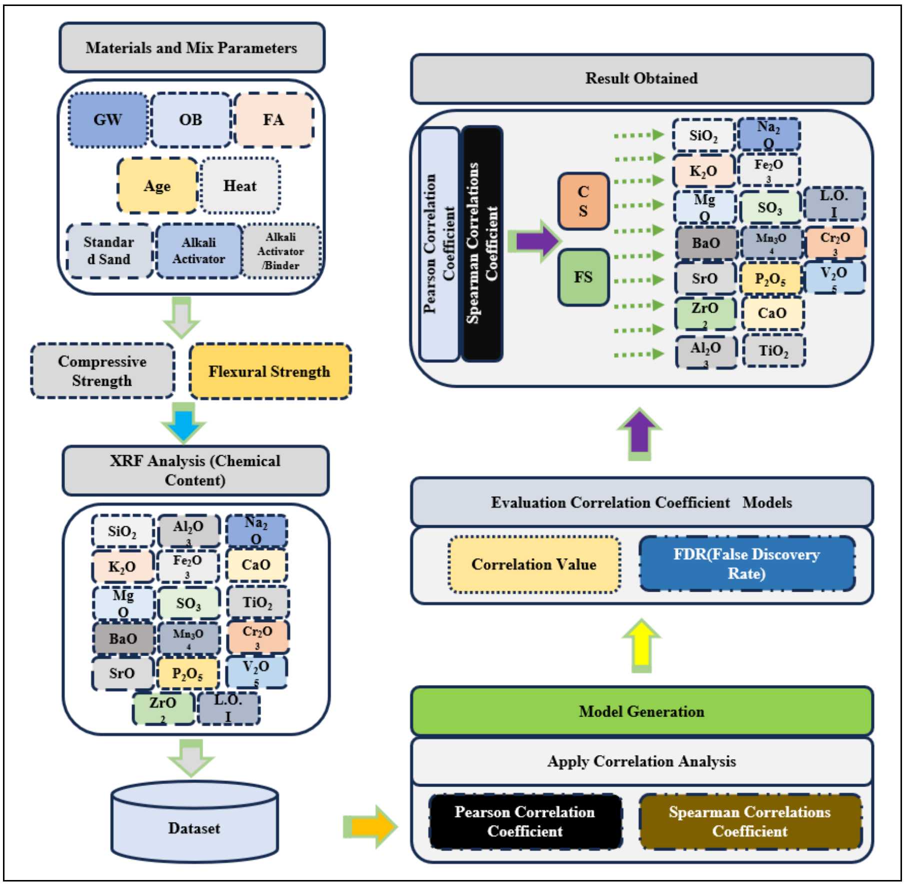

Figure 2. Flow diagram showing the stages of correlation analysis methods with the parameters that make up the dataset.

Table 1. Oxide compositions of obsidian, Fly Ash, and glass waste.

Oxide composition	Obsidian	Glass Waste	**Fly Ash**
SiO_2	73.624	70.938	58.921
Al_2O_3	13.779	1.997	22.357
K_2O	5.296	0.614	2.958
Na_2O	3.959	12.945	0.614
Fe_2O_3	1.263	0.22	6.357
CaO	1.044	8.537	3.264
TiO_2	0.207	0.17	1.016
BaO	0.083	-	0.149
MgO	0.075	3.664	1.818
Mn_3O_4	0.055	0.01	0.076
SO_3	0.022	0.302	0.211
P_2O_5	0.02	0.005	0.345
SrO	0.018	-	0.09
L.O.I.	0.510	0.600	1.7

Table 2. Mixture calculations.

Mixes	Binder			Sand (g)	Alkali Activator (g)	Alkali Activator/Binder
	OB (g)	GW (g)	FA (g)			
OB 100	450	0	0	1350	202.5	0.45
GW 100	0	450	0	1350	202.5	0.45
FA 100	0	0	450	1350	202.5	0.45
OB75GW25	337.5	112.5	0	1350	202.5	0.45
OB75FA25	337.5	0	112.5	1350	202.5	0.45
OB25FA75	112.5	0	337.5	1350	202.5	0.45
GW50FA50	0	225	255	1350	202.5	0.45
GW25FA75	0	112.5	337.5	1350	202.5	0.45
OB25GW75	112.5	337.5	0	1350	202.5	0.45
GW75FA25	0	337.5	112.5	1350	202.5	0.45
OB50FA50	225	0	225	1350	202.5	0.45
OB50GW50	225	225	0	1350	202.5	0.45

Each specimen was first broken in the flexural test and two compressive strength values were obtained, one flexural strength and one compressive strength from the broken pieces. The mortar specimens were kept in room conditions for 24 hours after casting and allowed to set. At the end of 24 hours, they were kept in an oven at 90 °C for 72 hours for curing. After 72 hours, the samples taken from the oven were kept in locked airtight bags under room conditions until the day of fracture. Mechanical properties such as compressive and flexural strengths obtained from the fractured specimens constituted the dataset. XRF analyses were performed on the crushed samples, and their chemical contents were obtained. The laboratory processes that enable the formation of the dataset are given in Figure 1.

2.3 Method

2.3.1 Correlation methods

Pearson and Spearman correlation coefficients used in this study are two different methods used in statistical analyses and are used to evaluate the strength and direction of the relationship between two variables.

2.3.1.1 Pearson correlation method

Pearson correlation method measures the linear relationship between two continuous variables [37]. It determines how strong and in which direction the relationship between the variables is. Pearson correlation coefficient value varies between -1 and 1: 1 means there is a perfect positive correlation, 0 means there is no relationship, while -1 means there is a perfect negative correlation.

2.3.1.2 Spearman correlation method

The Spearman correlation coefficient measures how strong the relationship between two variables is in a monotonic (continuously increasing or decreasing) manner. It is based on the ordering of the variables and does not require the assumption of normality [38]. The Spearman correlation coefficient also takes a value between -1 and 1. "Correlation for Compressive Strength" and "Correlation for Flexural Strength" in the data represent the correlations of different properties between these two different measurements. The "FDR Value" represents the false discovery rate. These values are used to check statistical significance. FDR is a method used to check the type of error that occurs when multiple comparisons are made in statistical tests. When many hypothesis tests are performed, the probability of obtaining randomly significant results increases. FDR is used to control and correct such false positive results. Pearson and Spearman correlation coefficients and FDR values given in Tables 3 and 4 are statistical analysis results used to evaluate the strength and statistical significance of the relationship between variables. Both correlation coefficients offer different approaches to assess the relationship between variables, and which method to use is determined depending on the characteristics of the data and the purpose of the analysis.

Table 3. Pearson and spearman coefficient correlation compressive strength FDR value.

Feature	Pearson Coefficient Correlation-FDR	Spearman Coefficient Correlation-FDR
CS-OB	0.123	0.032
CS-FA	0.009	0.012
CS-GW	0.634	0.828
CS-SiO_2	0.185	0.133
CS-CaO	0.917	0.828
CS-Na_2O	0.595	0.538
CS-Al_2O_3	0.280	0.133
CS-MgO	0.698	0.491
CS-Fe_2O_3	0.180	0.162
CS-P_2O_5	0.011	0.014
CS-TiO_2	0.015	0.041
CS-Cr_2O_3	0.038	0.088
CS-ZrO_2	0.058	0.032
CS-SrO	0.086	0.032
CS-V_2O_5	0.195	0.053
CS-K_2O	0.634	0.491
CS-SO_3	0.748	0.940
CS-Mn_3O_4	0.872	0.538
CS-BaO	0.872	0.935
CS-L.O.I.	0.985	0.791

Table 4. Pearson and spearman coefficient correlation flexural strength FDR value.

Feature	Pearson Coefficient Correlation-FDR	Spearman Coefficient Correlation-FDR
FS-OB	0.097	0.323
FS-FA	0.227	0.160
FS-GW	0.731	0.893
FS-SiO_2	0.566	0.784
FS-CaO	0.641	0.644
FS-Na_2O	0.902	0.817
FS-Al_2O_3	0.731	0.406
FS-MgO	0.641	0.893
FS-Fe_2O_3	0.566	0.644
FS-P_2O_5	0.232	0.264
FS-TiO_2	0.598	0.859
FS-Cr_2O_3	0.902	0.893
FS-ZrO_2	0.227	0.105
FS-SrO	0.318	0.323
FS-V_2O_5	0.566	0.323
FS-K_2O	0.612	0.893
FS-SO_3	0.034	0.105
FS-Mn_3O_4	0.464	0.817
FS-BaO	0.566	0.853
FS-L.O.I.	0.227	0.105

3 Result and discussion

3.1 Compressive strength

Figures 3 and 4 show the results of Pearson and Spearman correlation analyses for compressive strength. Spearman correlation analysis results show that the highest positive correlation coefficient for compressive strength is with OB (r=0.726), while the lowest positive correlation is with SO_3 content (r=0.025). This is also evidenced by the compressive strength values. It is seen that the compressive strength increases as the OB content increases. In addition, negative correlation for compressive strength occurred with FA (r=-0.841). The minimum negative correlation occurred for BaO (r=-0.046). The results of Pearson correlation analysis show that the highest positive correlation coefficient for compressive strength was with Cr_2O_3 (r=0.725), while the lowest positive correlation was with L.O.I content (r=0.006).

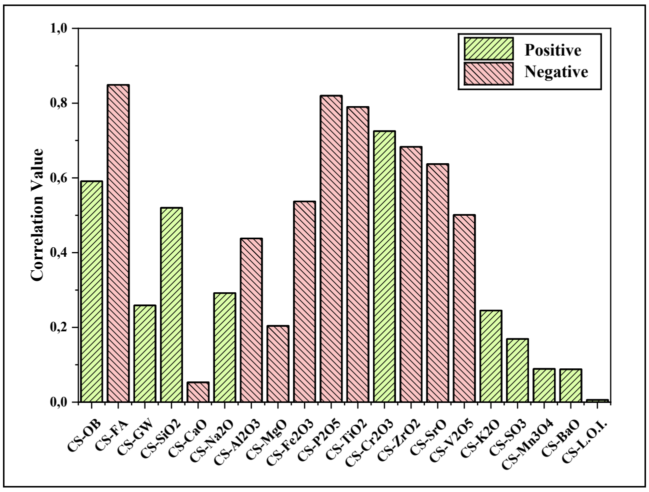

Figure 3. Pearson coefficient correlation compressive strength correlation value methods.

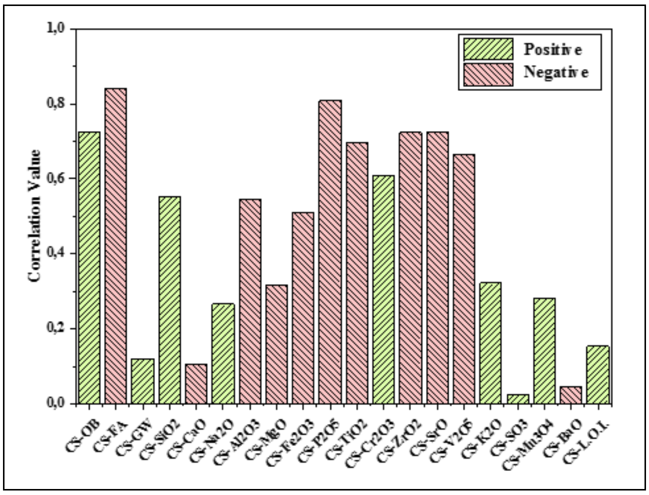

Figure 4. Spearman coefficient correlation compressive strength correlation value.

In addition, the maximum negative correlation for compressive strength occurred with FA (r=-0.849). The minimum negative correlation occurred for CaO (r=-0.053). These values show that the correlation coefficient analysis results obtained for compressive strength are very close to each other for both methods (Relative difference <1%). Pearson and Spearman coefficient correlation analysis compressive strength FDR values are given in Table 3. In contrast to the classical approaches found in statistical science, multiple hypothesis testing takes a more logical approach by using different analyses such as FDR. FDR is defined as the ratio of false positives to all positives and is expressed as the tentative rejection of a null hypothesis or the tentative acceptance of an alternative hypothesis [39],[40].

3.2 Flexural strength

Figures 3 and 4 depict the results of Pearson and Spearman correlation analyses between the chemical compositions and compressive strength, respectively. Figures 5 and 6 represent the results of Pearson and Spearman correlation analyses for flexural strength. The Spearman correlation analysis results show that the highest positive correlation coefficient for compressive strength was with L.O.I. (r=0.734), while the lowest positive correlation was with GW content (r=0.044).

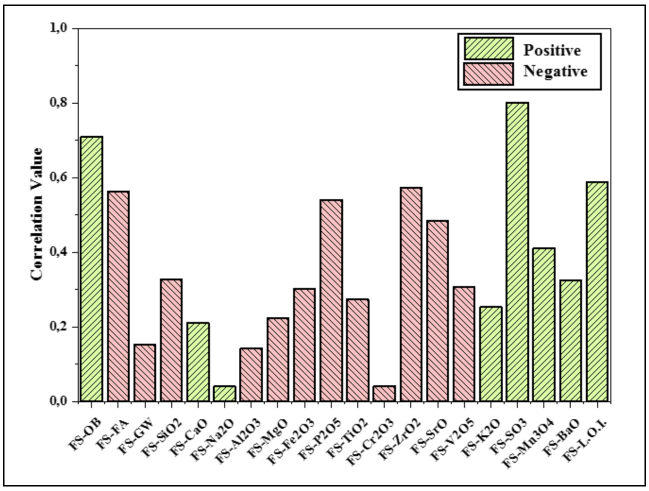

Figure 5. Pearson coefficient correlation flexural strength correlation value.

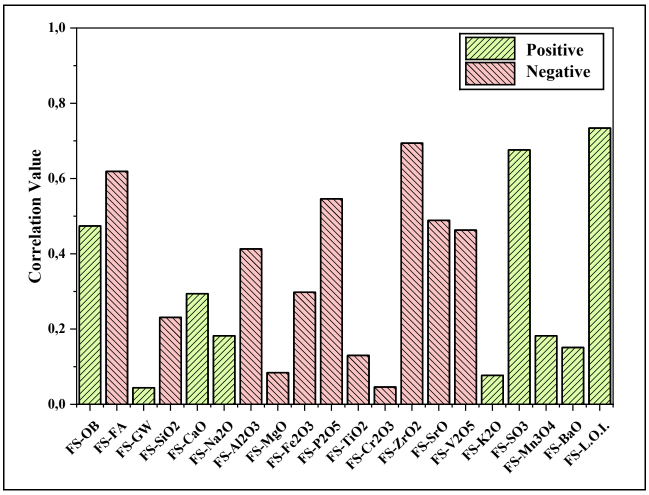

Figure 6. Spearman coefficient correlation flexural strength correlation value.

In addition, the maximum negative correlation for compressive strength occurred with ZrO_2 (r=-0.694). The minimum negative correlation occurred for Cr_2O_3 (r=-0.046). The results of Pearson correlation analysis confirm that the highest positive correlation coefficient for compressive strength is with SO_3 (r=0.802), while the lowest positive correlation is with Na2O content (r=0.040). In addition, the maximum negative correlation for compressive strength occurred with ZrO_2 (r=-0.572). The minimum negative correlation occurred for Cr2O3 (r=-0.041). While the difference between the predictions of the two methods for compressive strength was less than 1%, this difference increased to 9.3% for flexural strength.

When the literature is examined, it is seen that the R^2 coefficient, which is the performance metric in compressive strength and flexural strength prediction studies, is approximately 10% higher for compressive strength than flexural strength. This result is quite consistent with the data of this study [41]. Li et al. [42] used Pearson and Spearman methods for the statistical evaluation of the linear and nonlinear relationship between hydration properties and strength. It is seen that the difference between the values of the two methods is less than 1%. The results of the flexural strength FDR values' Pearson and Spearman coefficient correlation analysis are shown in Table 4. The accuracy of the dataset's positives increases as this ratio decreases. The Pearson and Spearman coefficient correlation analysis results show significant differences when Table 4 is compared. This is thought to be due to the difference in the algorithms of the methods used.

4 Conclusions

This study investigated the relationship between different mineral constituents and mechanical strength properties such as CS and FS in detail. The results obtained by using statistical analysis methods such as Pearson Correlation Coefficient and Spearman Correlation Coefficient have contributed significantly to our understanding of the relationship between mineralogical components and mechanical strength parameters.

The results of the analyses reveal the existence of a strong positive linear relationship between lime (CaO) content and compressive strength. This finding indicates that the determination of lime content in the selection of building materials is a potential strategy for improving structural strength. Furthermore, the positive monotonic relationship between silica (SiO_2) content and flexural strength emphasises the importance of considering silica content in the design of structural components. The results indicate that the combined evaluation of mineralogical constituents and mechanical strength properties in the building materials industry and civil engineering field can be an effective strategy for improving structural performance. Future studies may include a more comprehensive analysis of the data obtained with more material samples and experiments under different conditions.

This study has contributed to a better understanding of the role of mineral components in structural design and material selection processes. Further research is considered to have a great potential to contribute to applications in civil engineering and how to optimize structural strength.

5 Author contribution statement

Within the scope of this study, Yıldıran Yılmaz contributed to the investigation, methodology, and formal analysis of this article. Talip Çakmak contributed to methodology and obtained visualization. Zafer Kurt contributed to investigation, of this article and studied about writing - review & editing. İlker Ustabaş contributed to resources and supervision parts.

6 Ethics committee approval and conflict of interest declaration

“Ethics committee permission is not required for the prepared article”.

“There is no conflict of interest with any person/institution in the prepared article”.

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