Pamukkale Üniversitesi Mühendislik Bilimleri Dergisi

Pamukkale University Journal of Engineering Sciences

Assessment of thermal conductivity of rocks using regression analyses and artificial neural networks

Kayaçların termal iletkenliğinin regresyon analizleri ve yapay sinir ağları kullanılarak değerlendirilmesi

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Received/Geliş Tarihi: 06.12.2022 Revision/Düzeltme Tarihi: 10.05.2023 doi: 10.5505/pajes.2023.71609
Accepted/Kabul Tarihi: 30.08.2023 Research Article/Araştırma Makalesi

Abstract

This study investigated the thermal conductivity of natural stones (k) through regression analyses and artificial neural networks (ANN). In order to gather a sizable number of datasets for the aforementioned analytic methodologies, a thorough literature review was carried out. Based on different physicomechanical rock characteristics, like dry density (ρ_d), effective porosity (n_e), uniaxial compressive strength (UCS), and pulse wave velocity (V_p), seven estimated models (M1–M7) were created for the evaluation of k. The regression-based models (M1–M5) demonstrated that the considered rock properties influence the k of natural stones at different degrees. Notably, the n_e and V_p were found to be highly correlative parameters for estimating the k of natural stones. A number of statistical indicators were used to assess the performance of the developed models. The statistical evaluations indicated that the ANN-based models (M6, M7) provided more consistent results than the M1–M5 models. In addition, the mathematical expressions for ANN-based models were also given in the present study to let users carry out them more efficiently. In this case, this study is thought to ensure applicable and comprehensible information on the heat conduction of natural stones and can be described as a research study on how to model the k of natural stones as a factor of various rock characteristics.

Keywords: Thermal conductivity, natural stone, regression analysis, artificial neural networks

Öz

Bu çalışma, doğal taşların (k) termal iletkenliğini regresyon analizleri ve yapay sinir ağları (YSA) yoluyla araştırmıştır.Bu amaçla, yukarıda belirtilen analiz yöntemleri için çok sayıda veri seti derlemek için kapsamlı bir literatür araştırması yapılmıştır. Kuru yoğunluk (ρ_d), etkin gözeneklilik (n_e), tek eksenli basınç dayanımı (UCS) ve darbe dalga hızı (V_p) gibi farklı fizikomekanik kaya özelliklerine dayanarak, k'nin değerlendirilmesi için yedi tahmin modeli (M1–M7) kurulmuştur. Regresyona dayalı modeller (M1–M5), dikkate alınan kaya özelliklerinin doğal taşların k değerini farklı derecelerde etkilediğini göstermiştir. Özellikle, n_e ve V_p'nin doğal taşların k'sini tahmin etmek için yüksek oranda bağıntılı parametreler olduğu bulunmuştur. Kurulan modellerin performansı da çeşitli istatistiksel göstergeler kullanılarak değerlendirilmiştir. İstatistiksel değerlendirmeler, YSA tabanlı modellerin (M6, M7) M1–M5 modellerinden daha tutarlı sonuçlar verdiğini göstermiştir. Ayrıca, kullanıcıların bunları daha verimli bir şekilde uygulayabilmeleri için YSA tabanlı modeller için matematiksel ifadeler de bu çalışmada verilmiştir. Böylelikle, bu çalışmanın, doğal taşların ısı iletimi hakkında pratik ve anlaşılır bilgiler sağlayacağı düşünülmektedir ve farklı kaya özelliklerinin bir fonksiyonu olarak doğal taşların k'sının nasıl modelleneceğine dair bir vaka çalışması olarak tanımlanabilir.

Anahtar kelimeler: Isı iletkenliği, doğal taş, regresyon analizi, yapay sinir ağları

1 Introduction

The thermal properties of natural stones have been considered a critical research subject in earth sciences and geotechnical engineering. In this regard, the thermal conductivity of natural stones is of prime importance in numerous engineering fields such as heating and cooling systems in natural buildings, hydraulic characterization of aquifers, underground oil and natural gas investigations, design of buried high-voltage power cables, and nuclear waste storage systems [1]–[5]. In general terms, Thermal conductivity is a physical indicator of a material's ability to transmit temperature at the molecular level. From the rock mechanics perspective, it is denoted by k or λ (W/mK).

The thermal resistance of rocks is a function of k, a critical phenomenon for natural building stones. The higher the thermal resistance of rocks, the lower is the heat loss in the building. In that context, lower k values are desired for rocks, which are to be used as cladding and facing stones [6]. The k of natural stones is associated with various physical, chemical, and thermodynamical properties, such as mineralogical composition, thermal expansion of rock-forming minerals, porosity, and water content [7],[8]. The k is also a sensitive parameter to rock anisotropy [9]–[11].

Regarding modern rock mechanics and rock engineering approaches, one of the preferable methods to determine the k of intact rocks in the laboratory is based on the study by Popov et al. [3]. Furthermore, extensive experimental effort has been done in the last several decades to discover correlations between the k and other rock parameters. The results obtained from these studies provided comprehensive knowledge on the heat conduction of natural stones. For instance, Zimmermann [12] reported a statistically significant correlation between the k and n_e of rocks, where higher n_e values indicate higher thermal resistance [13]. However, it should be noted that rocks with higher n_e values have lower strength properties. In

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addition to the n_e, rock mineralogy can also be a critical factor affecting the k [14].

Uğur and Toklu [15] investigated the variations in physicomechanical rock properties such as effective porosity (n_e), k, water vapor transmission rate (WVTR), pulse wave velocity (V_p), and point load strength (PLS) due to various freeze-thaw cycles. The study demonstrated that rock lithology is a significant factor for evaluating the heat conduction of natural stones. More profoundly, the resistance of rocks to freeze-thaw cycles is mainly associated with the k of rocks. Yaşar et al. [16] investigated the relationships to estimate k, focusing on different characteristics of rocks, including their uniaxial compressive strength (UCS), V_p, dry density (ρ_d), and effective porosity (n_e). Focused on 25 different rock types from Turkey, they found significant relationships between the k and UCS, n_e, and V_p of rocks. Barry-Macaulay et al. [17] concluded that the k of soils and rocks increases in parallel with the ρ_d and humidity content. Demirci et al. [18] performed detailed laboratory investigations on some rock types from Turkey and found that the k increases with confining pressure (σ_3) in triaxial compressive strength tests. Özkahraman et al. [19], Boulanouar et al. [20], and Xiong et al. [21] also stated that the n_e and V_p of natural stones are highly correlative parameters for evaluating the k. In addition, Shim et al. [22] emphasized rock-forming mineral contents as a decisive factor determining the k of rocks from the republic of Korea. According to their study, the k of igneous, metamorphic, and sedimentary rocks was found to be between 2.80–4.24 W/mK, 2.87–6.08 W/mK, and 3.13–3.83 W/mK, respectively. Chen et al. [23] also reported that the k of rocks decreases with increasing ambient temperature.

The studies mentioned above demonstrated practical and straightforward approaches for evaluating k. However, the determination of k in laboratory is challenging, time-consuming, and expensive due to special equipment requirements and complicated testing methodologies. As a result, useful suggestions have been made to calculate the k of various rock materials. These theories or models are mainly based on regression analysis with relatively small-scale datasets. Apart from the studies by Singh et al. [24], Khandelwal [25], and Verma et al. [26], soft computing tools have not been regarded to predict the k of natural stones due to the limited datasets with different rock properties. Therefore, to contribute to the scientific literature on the thermal properties of natural stones, a thorough review of the literature was made to compile such datasets composed of different rock types and properties. In addition to the regression analyses, artificial neural networks (ANN) were adopted to predict the k of natural stones in this article.

Seven different predictive models (M1–M7) were established based on the above analysis methods. This paper presented the statistical performance evaluations of the models and various statistical criteria were used to test the efficiency of the developed models.

2 Data documentation

A thorough literature review was used to compile such datasets for the regression and soft computing investigations. Accordingly, different k values for various natural stones documented in the previous literature are plotted in Fig 1. Although there is immense literature on the thermal properties of rocks, most of the surveyed papers have limited information on the k as a function of the physicomechanical properties of rocks. Therefore, the studies whose data was adopted in this study were marked with a red star in Fig 1. The range of the datasets and considered rock properties are listed in Table 1. The considered independent variables in this study are the ρ_d, n_e, UCS and V_p. On the other hand, the dependent variable is k for regression and soft computing analyses.

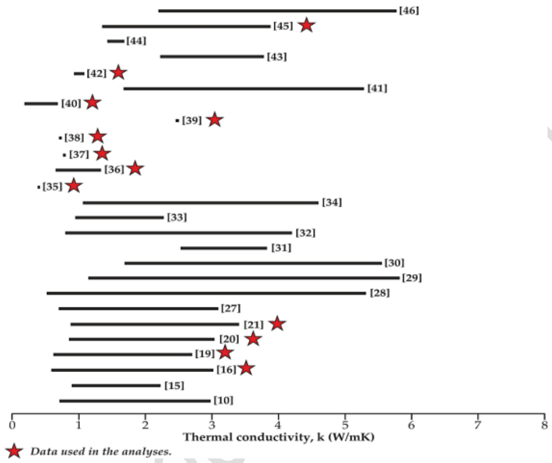

Figure 1. Different k values for various natural stones documented in previous literature.

3 Data analysis methods

In the context of the methods to estimate the k, single, multiple, and nonlinear regression analyses were first conducted. Then, ANN analyses were performed using the statistically correlative parameters. The details on these methods are given in the following subsections.

3.1 Regression analysis

In statistical modeling, regression analyses are one of the most straightforward procedures for revealing relationships between dependent and independent variables. However, based on their structural differences, they can be split into two categories. On the one hand, linear regression analyses, which can be either single or multiple, are mainly adopted considering small-scale datasets [47]. On the other hand, nonlinear regression analyses can also be considered for complex problems with a wide range of independent variables [48]. In this study, linear and nonlinear regression analyses were attempted to estimate the k of considered rocks. According to findings of the regression analysis, it was determined that the k could be simply modeled by linear and nonlinear models, which are given in Table 2. However, the regression-based predictive models (M1–M5) yielded correlation of determination (R^2) values ranging from 0.39 – 0.61. Therefore, it can be claimed that M1–M5 models have some limitations in estimating the k with high accuracy.

It means that the regression-based models established in this study provide some correlative parameters for the evaluation of k. Furthermore, it should be herein mentioned that the number of samples should be increased for the M3 model to obtain general inferences on how the UCS acts on the k. In summary, the results of the regression analysis showed that the investigated rock properties (ρ_d, n_e, UCS and V_p) can be explained as correlation parameters for the evaluation of k. Of these parameters, the ρ_d, n_e, and V_p with different coupling variables were considered for ANN analyses because the determination of these parameters is relatively simple in the laboratory.

Table 1. Descriptive statistics of the variables considered in this study.

Reference	Rock type	ρ_d (g/cm^3)	n_e (%)	UCS (MPa)	V_p (km/s)	k (W/mK)	n
[16]	Limestone, Sandstone, Siltstone, Marble, Dolomite, Basalt, Travertine, Andesite	2.24 – 2.97	0.86 – 3.05	33.20 – 120.80	2.95 – 6.30	0.59 – 3.01	25
[19]	Limestone, Travertine, Andesite	2.24 – 2.69	1.82 – 16.00	44.00 – 84.80	3.60 – 6.30	0.64 – 2.70	4
[20]	Sandstone, Travertine, Marble, Granite	N.R	0.25 – 35.83	N.R	3.07 – 6.00	0.87 – 3.03	13
[21]	Sandstone, Siltstone, Limestone, Dolomite, Mudstone, Shale	2.26 – 2.69	0.19 – 11.65	N.R	1.80 – 6.33	0.82 – 3.38	36
[35]	Tuff	1.40	40.00	9.00	2.30	0.40	1
[36]	Tuff, Basalt	1.35 – 2.74	1.83 – 29.47	17.65 – 175.19	1.52 – 4.76	0.64 – 1.33	6
[37]	Limestone	1.85	21.93	23	3.21	0.78	1
[38]	Limestone	1.89	25.93	20	3.27	0.72	1
[39]	Granite	2.65 – 2.66	0.56 – 0.71	N.R	N.R	2.45 – 2.49	7
[40]	Ignimbrite	1.04 – 2.11	11.20 – 51.00	N.R	N.R	0.18 – 0.68	4
[42]	Claystone	1.94 – 2.27	34.00 – 42.00	N.R	N.R	0.93 – 1.08	4
[45]	Travertine, Andesite	2.37 – 2.68	0.16 – 4.92	N.R	N.R	1.35 – 3.88	3

ρ_d: Dry density, n_e: Effective porosity, UCS: Uniaxial compressive strength, V_p: Pulse wave velocity, k: Thermal conductivity, n: Number of samples, N.R: Not reported.

Table 2. Empirical formula to estimate the k of rocks.

Model No	Empirical formula	Estimate	SE Estimate	t value	Number of datasets, n	R^2
M1	$k = \exp(-2.1298 + 1.073\,\rho_d)$	−2.1298 1.073	0.4815 0.1838	−4.423 5.837	92	0.39
M2	$k = -0.4485\ln(n_e)+2.2688$	−0.4485 2.2688	0.0414 0.0768	10.833 29.541	105	0.53
M3	$k = \dfrac{6.434UCS}{241.99 + UCS}$	6.434 241.99	3.343 168.044	1.924 1.440	38	0.58
M4	$k = -0.3797 + 0.5179V_p$	−0.3797 0.5179	0.207 0.0481	1.834 10.797	87	0.58
M5	$k = 0.429{n_e}^{-0.077}{V_p}^{1.032}$	0.429 −0.077 1.032	0.1268 0.0368 0.1801	3.383 −2.092 5.7301	87	0.61

3.2 Artificial neural networks (ANN)

Artificial neural networks (ANNs) are one of the deep learning algorithms developed by imitating the biological nervous system in the human brain. It can be defined as a parallel distributed processing algorithms [24] and are commonly used to estimate multiple dependent variables based on complex datasets. In this study, a few neural networks were created using the neural network toolbox (nntool) in the

MATLAB software. The database was randomly split into training (70/100) and testing (30/100) sections before being used in the soft computing analysis. To find the most appropriate and useful structural arrangement, a variety of potential network designs with varying hidden layers and neurons were tested. Prior to executing the ANN analyses, the datasets were normalized by Eq 1 to minimize the problems arising from overfitting [49, 50].

$$V_N = 2\left(\frac{X_i - X_{min}}{X_{max} - X_{min}}\right) - 1 \qquad (1)$$

where x_i is the essential variable to be standardized, in the dataset, x_{min} is the minimum value while x_{max} is the maximum value (Table 1).

In a neural network model's architecture, activation functions are crucial, and choosing the right activation function can significantly enhance the neural network's performance. Three activation functions, which are Rectified Linear Activation (ReLU), Logistic (Sigmoid), Hyperbolic Tangent (Tanh), are the most commonly used [51]. Finding the most important features in the data sets with the tanh activation function appears the most efficient method [52].

A feedforward backpropagation algorithm with Levenberg-Marquardt training function, which is the most efficient method, is used to train neural networks. As shown in Equation 2, the Tangent sigmoid (tanh) function was used to transmit data via neurons.

$$tanh = \frac{2}{1 + e^{-2x}} - 1 \qquad (2)$$

An input layer, an output layer, and at least one hidden layer are features of a typical backpropagation network. Yet, there is no theoretical restriction on the number of hidden layers [53]. How many hidden layers will be used in neural networks and how many neurons will be in each hidden layer have not been determined until now. These characteristics, which change depending on the issue, are discovered through trial and error [54]. For estimating the k, the optimal and practical ANN structures were found to be 2–6–1 and 3–6–1, respectively (Fig 2). After the ANN has been trained, by utilizing the weights and biases predicted equations can be created. On this subject, the empirical models (M6–M7) to estimate k can be derived using Eq 3 [26, 55].

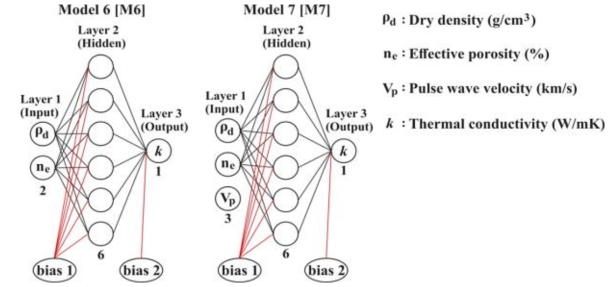

Figure 2. ANN structures considered in this study.

$$y_1 = f_0\{W_0[f_i(w_i \times x_i + B_i)]+B_0\} \quad (3)$$

where f_0 and f_i are the transfers functions. Additionally, the weight vectors of the output and input layers are designated by W_0 and W_i, respectively, and the bias vectors of the output and input layers are designated by B_0 and B_i, respectively. The normalized input parameter is called x_i(Eq 2).

Based on the above explanations, the empirical models to estimate k are given by Eq 4 and Eq 5. The sub-equation systems for the above equations are given in Table 3.

For Model 6 (M6)

$$k = 1.85\, tanh\left(\sum_{i=1}^{6} A_i - 0.33918\right) + 2.03, R^2 = 0.79 \quad (4)$$

For Model 7 (M7)

$$k = 1.49\, tanh\left(\sum_{i=1}^{6} S_i - 0.19217\right) + 1.89, R^2 = 0.88 \quad (5)$$

Table 3 Sub-equation systems for the developed ANN models.

Model 6 [M6], Number of datasets, n = 92
$A_1 = 6.937tanh(-5.0585^n\rho_d + 14.7519^n n_e + 16.8968)$
$A_2 = 8.5624tanh(-2.2697^n\rho_d + 15.9481^n n_e + 15.0427)$
$A_3 = -3.8189tanh(-126641^n\rho_d + 2.9962^n n_e + 10.7458)$
$A_4 = 2.2153tanh(-10.4769^n\rho_d - 0.55813^n n_e + 6.1312)$
$A_5 = -0.78126tanh(-3.8004^n\rho_d + 1.8582^n n_e - 3.7634)$
$A_6 = -15.0663tanh(-1.9354^n\rho_d + 10.4007^n n_e + 10.4155)$
Normalization functions
$n_{\rho_d} = 1.0363\rho_d - 2.0777$
$n_{n_e} = 0.0393n_e - 1.0063$
Model 7 [M7], Number of datasets, n = 74
$S_1 = (2.3369tanh(-2.7754^n\rho_d + 1.328^n n_e + 4.3425^n V_p + 2.971)$
$S_2 = 1.6008tanh(-3.4719^n\rho_d + 4.8584^n n_e - 2.7414^n V_p + 3.6805)$
$S_3 = 2.8501tanh(-5.6677^n\rho_d - 5.0167^n n_e + 0.40374^n V_p - 0.8289)$
$S_4 = -5.7143tanh(-3.1955^n\rho_d - 2.2601^n n_e + 1.7612^n V_p + 0.09401)$
$S_5 = -2.4581tanh(-7.8283^n\rho_d - 1.1693^n n_e + 6.2002^n V_p - 0.64219)$
$S_6 = -3.9039tanh(1.1339^n\rho_d - 1.5101^n n_e - 3.6895^n V_p + 0.29946)$
Normalization functions
$n_{\rho_d} = 1.2308\rho_d - 2.6554$
$n_{n_e} = 0.0502n_e - 1.0095$
$n_{V_p} = 0.4158V_p - 1.632$

4 Results and discussion

The regression analysis results demonstrated that the considered rock properties (ρ_d, n_e, UCS, V_p) are associated with the k of rocks. However, for a large number of datasets, the models based on these parameters yielded relatively lower R^2 values, which ranged from 0.39 to 0.61 (Fig 3). The underlying reason for obtaining relatively lower R^2 values for the regression-based models (M1–M5) can be attributed to the fact that these models were established based on a relatively large number of datasets with different rock origins. For example, for small-scale datasets (n=6), Yüksek [36] found stronger relationships ($R^2 > 0.93$) to estimate the k as a function of ne and V_p.

In another study by Özkahraman et al. [19], the k was estimated with high accuracy ($R^2 > 0.97$), using five datasets (n=5). Similar strong correlations ($R^2 > 0.85$) were also reported by Boulanouar et al. [20], who used 13 datasets (n=13) to estimate the k of rock from Morocco.

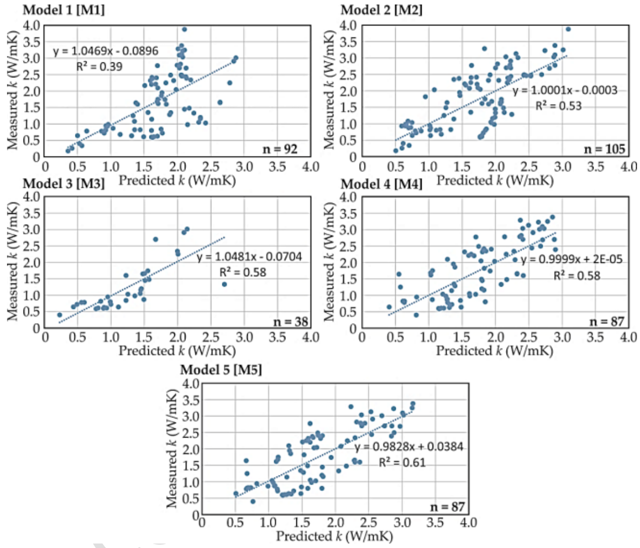

Figure 3. Predicted and measured k values for the regression-based models (M1–M5).

In contrast, when increasing the number of samples in the regression analyses to estimate the k of rocks, R^2 values tend to decrease, as Xiong et al. [21] stated. For the mentioned study, the k was modeled as a function of ne using 36 datasets composed of different sedimentary rocks. The R^2 value of this model was about 0.57. When it comes to the ANN analysis results, the R^2 values for the M6 and M7 models were determined as 0.79 and 0.88, respectively (Fig 4). In the M6 model, ρ_d and n_e were considered together, whereas the V_p was integrated into the M6 model, which is called M7 (Fig 2). This new model yielded more consistent results in estimating the k of rocks. Hence, multilayer feedforward networks with suitable correlative parameters (e.g., n_e and V_p) can be considered an accurate representation of input-output relationships in the ANN analyses [24].

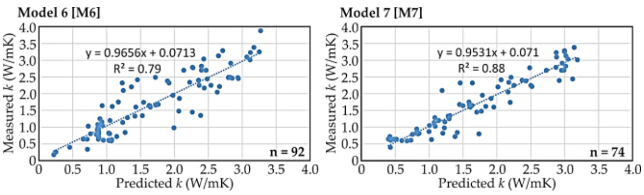

Figure 4. Predicted and measured k values for the ANN-based models (M6–M7).

Several statistical indicators, including root means squared error (RMSE), mean absolute percentage error (MAPE), and the variance accounted for (VAF) were also used to assess the performance of the established models. The equations to calculate the above indices are given in Eqs. 6 – 8.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(o_i - e_i)^2}{n}} \quad (6)$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}|o_1 - e_i| \quad (7)$$

$$VAF = (1 - \frac{var(o_i - e_i)}{var(o_i)}) \times 100 \tag{8}$$

where o_i is the observed data, e_i is the predicted data, and n is the number of observations.

The performance evaluation of the established predictive models are summarized in Table 4. Models that have been substantially more successful tend to have higher VAF and lower RMSE and MAPE values [56]. Accordingly, the M5 has the lowest relative errors, with RMSE and MAPE values of 0.531 and 0.454, respectively among the regression-based models and, the VAF for this model is 60.72. On the other hand, the M7 model yielded the best prediction performance among the models established in this study. The RMSE, MAPE, and VAF values for the M7 model are 0.309, 0.222, and 87.15, respectively. Conclusions

This paper aimed to propose such predictive models to estimate the k of rocks. For this aim, an extensive literature review was carried in order to gather these datasets for regression and ANN analysis. (Table 1). The outcomes of the regression analysis indicated that the ρ_d, n_e, UCS and V_p affect the k of rocks (Table 2). Using these variables, linear and nonlinear regression models (M1–M5) were established. However, their prediction capability is not enough for precise estimations. To obtain additional predictive models with higher prediction accuracy, such ANN analyses were performed. In the context of ANN analyses, the ρ_d, n_e, and V_p were considered (Fig 2) since the determination of these parameters is relatively simple in laboratory studies. Based on these analyses, the M6 and M7 models were developed. In addition, this study contains the mathematical equations for these models so that users may more effectively utilise them (Table 3). When the models created by using various statistical indicators were evaluated, it was concluded that the M7 model gave the best prediction performance among the models established in this study (Table 4). Therefore, it could be reliably used to evaluate the k of rocks. However, the number of datasets with different rock properties should be considered for further studies. In this regard, the current work is considered to offer plain and useful understanding on how rocks transport heat and can be proclaimed a case study on how to model the k of rocks in relation to various rock characteristics.

5 Acknowledgments

6 Author contribution statements

In the study, the first author created the hypothesis of the research, designed the methods to be used, created the models, literature review, discussion of the results, interpretation and article writing. The second author contributed to literature review, discussion and interpretation of results, and article writing. The researcher, who was not involved in the study as an author, contributed with her experience in models created using regression analyzes and artificial neural networks.

7 Ethics committee approval and conflict of interest statement

There is no need to obtain permission from the ethics committee for the article prepared.

There is no conflict of interest with any person or institution in the article prepared.

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Table 4. Performance evaluation of the established predictive models.

Data analysis method	Model No	R^2	RMSE	MAPE	VAF	Number of samples, n	Independent variables
Regression	M1	0.39	0.696	0.567	39.40	92	ρ_d
	M2	0.53	0.601	0.489	53.24	105	n_e
	M3	0.58	0.463	0.357	57.62	38	UCS
	M4	0.58	0.550	0.484	57.73	87	V_p
	M5	0.61	0.531	0.454	60.72	87	n_e, V_p
ANN	M6	0.79	0.407	0.308	79.29	92	ρ_d, n_e
	M7	0.88	0.309	0.222	87.15	74	ρ_d, n_e, V_p

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