Characterizing Shale Rock Properties Using Data Analytics with Vipulanandan Failure and Correlation Models

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ABSTRACT
With the increasing construction activities in shale rocks around the world related to transportation tunnels, support bridges, buildings, and storage facilities and also hydraulic fracking. In this study, over 180 data were used to characterize the shale rock behaviors including the statistical distributions of the data. The study included density, pulse velocity, permeability, and strength. The density of shale was in the range of 1.7 to 3.0 g/cm^3. The compressive strength and tensile strength of the rocks investigated varied up to 200 MPa and 9.5 MPa respectively. Vipulanandan correlation model was effective in relating the tensile strengths, fracture toughness and the compressive strength of the rock. The Mohr-Coulomb failure criteria is used to characterize the failure of the rocks and it overestimates the tensile strength and has no limit on the maximum shear strength tolerance for the rocks. The new Vipulanandan failure model was developed to not only better quantify the tensile strength but also to predict the maximum shear strength tolerance of the rocks The maximum shear stress (τmax.) for the shale was 102 MPa based on the collected data. Based on the coefficient of determination and the root mean square error values, the new Vipulanandan failure model predicted the results better than the Mohr-Coulomb model.

1. INTRODUCTION
It is necessary to better quantify the mechanical properties and failure criteria of the shale rocks to construct different types of infrastructure on the rocks (Mohammed and Mahmood, 2018 a). It is also important to design the drilling and fracturing processes using the rock properties, including the tensile strength and failure criteria, for hydraulic fracturing of rocks in a cost-effective way (Mohammed and Mahmood, 2018 b). To define the failure of the rocks, Mohr-Coulomb criteria is used with over prediction of the tensile strength and no limit on the maximum shear strength tolerance with the normal stress on the rocks applied (Singh et al., 2015; Vipulanandan and Mohammed, 2018; Mahmood et al., 2020; Vipulanandan 2021). Hence, there is a need to developing property correlations and improved the failure criteria of rocks since, there is very limited property correlation in the literature (Omar, 2017).

Shale is a fine-grained sedimentary rock composed of mud that is a mix of flakes of clay minerals and tiny fragments (silt-sized particles) of other minerals, especially quartz and calcite (Tucker 2009).

In rock engineering, most applied rock classification systems are based on mechanical parameters such as uniaxial unconfined compressive strength (UCS), tensile strength (σt), and Young's modulus or deformability modulus (E) (Selçuk and Nar 2016). Unconfined compressive strength (UCS), the most widely used property to evaluate rock strength, costly and time-consuming testing with sample preparation and testing (Karakus et al. 2005). Many researchers have introduced several empirical equations for the determination of rock strength from simple physical properties. Using such properties, rock strength may be determined in an easy, quick, and inexpensive manner during field investigations (Sabatakakis et al. 2008, Rajabzadeh et al. 2012). Tensile strength and fracture toughness are two important parameters in rock mechanics, and it is used in the initiation and propagation of fractures in hydraulic fracture modeling (Meng and Pan 2007, Vipulanandan and Mohammed 2014).

2. OBJECTIVES

Quantify the mechanical behavior of the shale rocks based on more than 180 data collected from previous research studies are the objective of this study. The main objectives are as follows:

1. To qualify the statistical variation in the density, compressive strength, and tensile strength of shale rocks.
2. Investigate and quantify the correlation relationship between the compression strength and tensile strength and fracture toughness of shale rocks using the Vipulanandan correlation model.
3. Quantify the shear failure strength for the rocks using the new Vipulanandan failure model and compared it with the Mohr-Coulomb model prediction.

3. METHODS AND MATERIALS

Data collection

This study focused on the behavior of the shale rock based on the data collected from several studies in the literature. The properties of interest were density, compressive, tensile strengths, fracture toughness of shale rock.

Modeling

Vipulanandan correlation model

Based on the inspection of the data collected, the correlation between the properties of shale rock was investigated using the Vipulanandan correlation model the relationship is as follows (Mohammed and Vipulanandan, 2014&2015; Mohammed and Mahmood, 2019; Mahmood and Mohammed, 2020; Ghafor et al., 2020 a&b; Vipulanandan 2021):

$$Y = Yo + \frac{X}{(A+B*X)} \tag{1}$$

where:

X= independed variables
Y= depended variable
A, B and Yo = model parameters depend on the rock property.
The results obtained from Eq. 1 were compared with the model (Eq. 2) which has been used in the literature (You, 2015).

$$Y = \propto * (X)^{0.5} \tag{2}$$

where α is the model parameter.

Failure models

(i) Vipulanandan failure model

Based on years of experience and reviewing the material shear strength versus applied normal stress is nonlinear, also there is a limit to the maximum shear stress tolerance for all the materials, and hence following model and conditions are proposed (Vipulanandan and Mohammed, 2018; Vipulanandan 2021):

$$\tau = \tau_o + \frac{\sigma_n}{C + D * \sigma_n} \tag{3}$$

when $\sigma_n \rightarrow \infty$

$$\tau_\infty = \tau_o + \frac{1}{D} \quad (4)$$

Hence, this model (Eq.4) has a limit on the maximum shear stress the rocks will tolerate at relatively high normal stress.

(ii) Mohr-Coulomb failure model

The linear relationship between the shear strength (τ) of a rock and the applied normal stress (σ_n) on the failure plane is represented by the Mohr-Coulomb failure criterion. This relation is as follows:

$$\tau = \tau_o + \sigma_n \tan \phi \quad (5)$$

where τ_o is the cohesion and the angle ϕ is called the angle of internal friction. From Eq. (5) when $\sigma_n \rightarrow \infty$; $\tau = \infty$. Hence, Mohr-Coulomb failure model does not satisfy the upper limit condition for the shear strength tolerance of the materials.

4. RESULT AND ANALYSIS

Statistical analysis

Density (γ)

Based on 184 data on shale rock collected from the literature, the mean value of density was 2.50 gm/cm^3 as summarized in Table 1 and shown in Figure 1. The density of shale rock varied from 1.70 gm/cm^3 to 3 gm/cm^3 based on 184 data the standard deviation was 0.248 gm/cm^3 and variance of 9.9% as summarized in Table 1. For the density of shale rock, Weibull distribution was selected based on AD and P-value testing as shown in Figure 1.

Table 1. Statistical parameters of geotechnical properties of rocks

Statistical Parameters	Density (gm/cm^3)	Compressive Strength, σ_c (MPa)	Tensile Strength, σ_t (MPa)
No. of Data	184	184	81
Range	1.7-3	2-200	2.5-9.5
Mean (μ)	2.5	61.90	6.8
Std. Deviation (σ)	0.248	35.28	1.156
Coefficent of Variation (COV)	9.9%	57%	17%

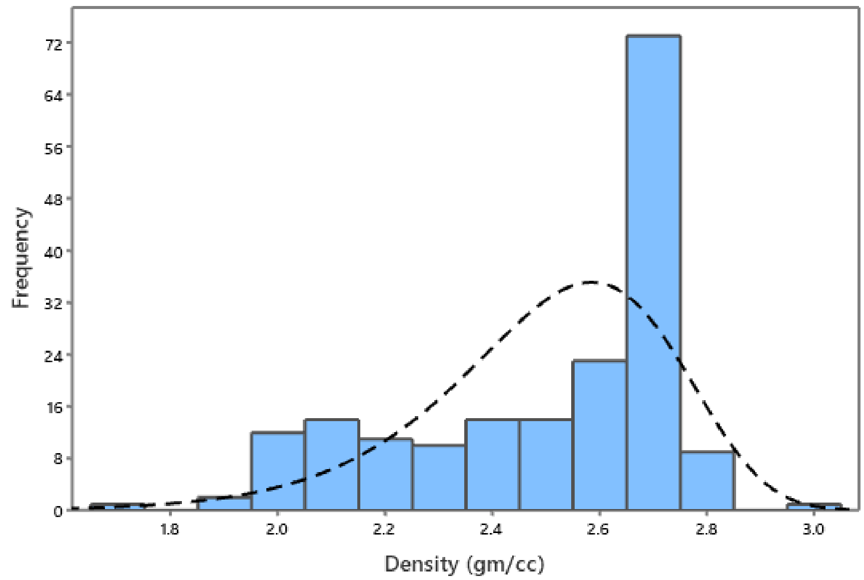

Figure 1. Density Distribution for the Shale Rock

Compressive strength

Based on more than 500 data of the limestone, sandstone, and shale rocks collected from the literature (Table 1, 2, and 3), the σ_c data for limestone varied from 2 MPa to 200 MPa with a median of 62.5 MPa, the SD of 35.69 MPa and variance of 1274 as summarized in Table 4. For the σ_c of limestone rock, 3-Parameter Weibull distribution was selected Based on AD and P-value testing (Fig. 1(b)). According to the 184 compressive strength for sandstone data from the literature (Table 2), the data varied from 19 MPa to 145 MPa with a median of 86.15 MPa, the SD of 32.9 MPa, and a variance of 1274 (Table 4). Based on 184 of σ_c data for shale rock, the data varied from 2 MPa to 201 MPa with a median of 61.9 MPa, the SD of 35.28 MPa, and coeifficient of varaion (COV) of 57% as summarized in Table 1. Based on AD and P-value testing,the compressive strength (σ_c) of shale rock was normaliy distributed as shown in Figure 2.

Tensile strength (σ_t)

Based on total of 81 tensile strength data for shale rock, the data varied from 2.5 MPa to 9.5 MPa with a median of 6.8 MPa, and standard deviation of 1.156 MPa. Based on AD and P-value testing, the tensile strength (σ_t) for the shale rock was 3-Parameter Weibull distribution as shown in Figure 3.

Property correlation

Relationship between Compressive strength (σ_c) and Density (γ)

Based on 184 data collected for shale rock, there was no direct correlation was between the density (γ) and compressive strength (σ_c) as shown in Figure 4.

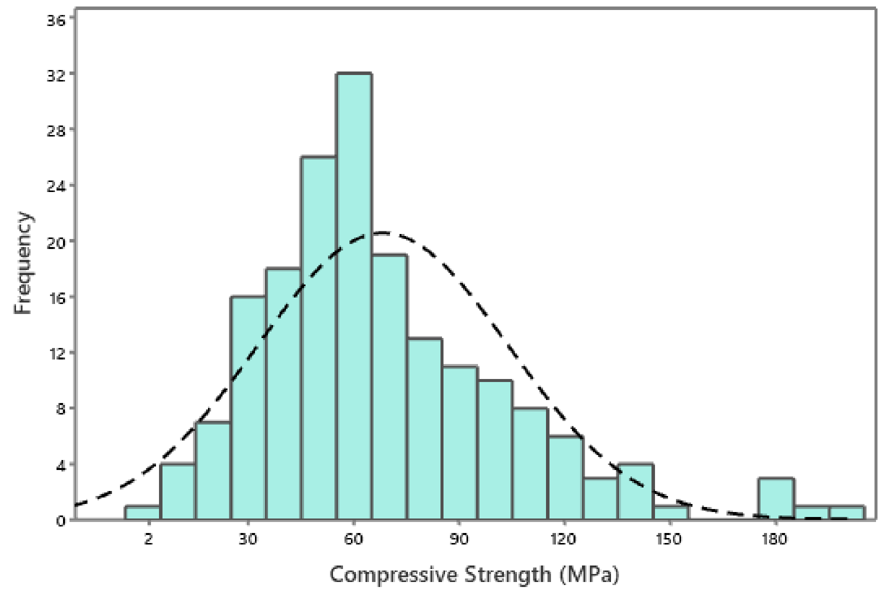

Figure 2 Compressive Strength Distribution for the Shale Rock

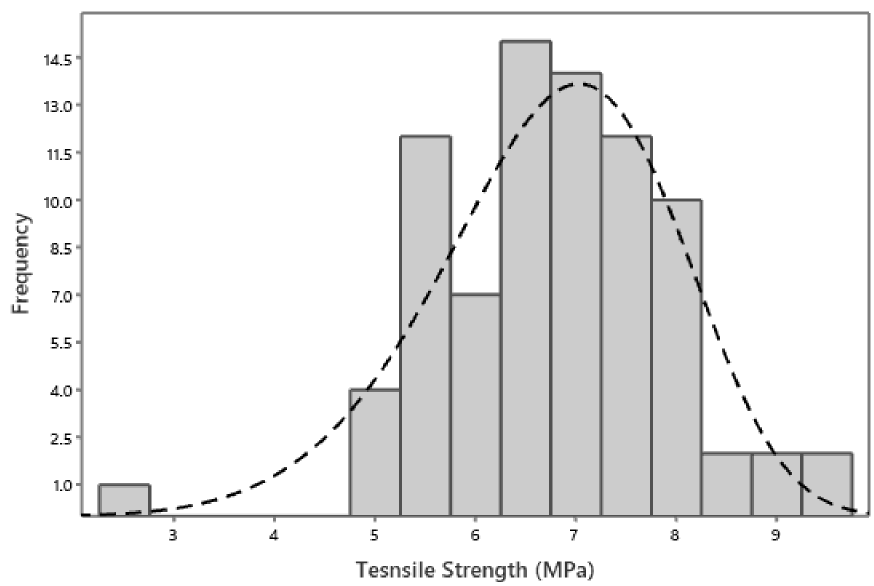

Figure 3 Tensile Strength Distribution for the Shale Rock

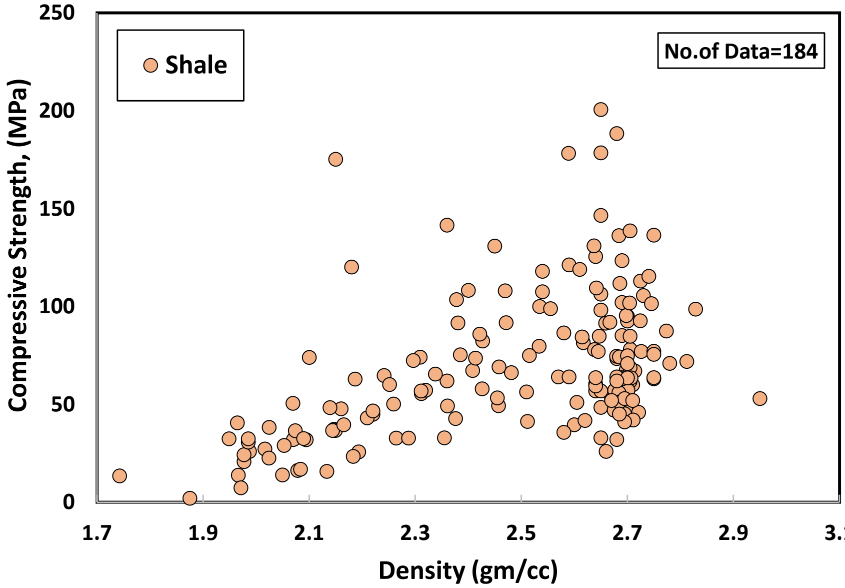

Figure 4 Compressive Strength and Density for the Shale Rock

Tensile strength (σ_t) and compressive strength (σ_c)

A total of 23 data were collected from the literature. With the increasing of σ_c of rocks, the σ_t nonlinearly also increased as shown in Figure 3. The change in the σ_c with σ_t of rocks was represented using the Vipulanandan correlation model relationship (Eq. 1) and the model parameters A, B, coefficient of determination (R^2), and root mean square error (RMSE) were 6.5, 0.075 MPa^{-1}, 0.97 and 0.32 MPa respectively as summarized in Table 2. With the increase in σ_c of the shale rock from 10 MPa to 100 MPa, the σ_t increased from 1.8 MPa to 8.5 MPa (Fig. 5(c)) when the rock compressive strength increased to 200 MPa as shown in Figure 5. The model results were compared with the model used in literature (Eq. 2), based on the coefficient of determination (R^2) and root mean square error (RMSE), the Vipulanandan correlation model predicted the relation between σ_c and σ_t better than the Eq.(2) as summarized in Table 2.

Table 2 Model parameters for tensile and compression strength relationship

			Model (Eq.2)			**Vipulanandan correlation model (Eq.1)**				
Depended Variable (Y-axis)	In depended Variable (X-axis)	Type of Rock	α	RMSE (MPa)	R^2	A	B MPa^{-1}	RMSE (MPa)	R^2	No. of Data
Tensile Strength, σt (MPa)	Compressive Strength, σc (MPa)	Shale	0.70	0.48	0.93	6.5	0.075	0.32	0.97	23

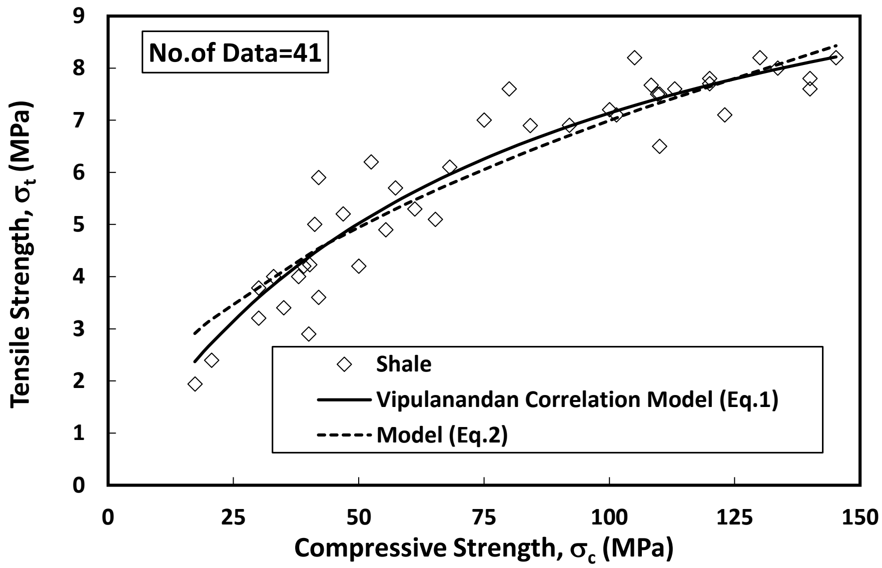

Figure 5 Correlation Between the Compressive Strength and Tensile Strength of the Shale Rock

Fracture Toughness (K_1) and Tensile Strength (σ_t)

The fracture toughness (K_1) of shale rock is nonlinearly increased as σ_t increased as shown in Figure 6. The correlation between K_1 and σ_t was investigated using the Vipulanandan correlation model (Eq. 1) and compared to other model used in the literature (Eq. 2) . The model parameters A, B, the coefficient of determination (R^2) and root mean square error (RMSE) were 4.96, 0.69, 0.88, and 0.085 MPa.m$^{0.5}$ respectively as summarized in Table 3. According to the coefficient of determination (R^2) and root mean square error (RMSE), the Vipulanandan correlation model predicted the relation between K_1 and σ_t better the Eq. 2 as summarized in Table 3.

Table 3. Model parameters for tensile strength and fracture toughness relationship

			Model (Eq.2)			**Vipulanandan correlation model (Eq.1)**				
Depended Variable (Y-axis)	In depended Variable (X-axis)	Type of Rock	α	RMSE (MPa)	R^2	A	B MPa^{-1}	RMSE (MPa. $m^{0.5}$)	R^2	No. of Data
Fracture Toughness (MPa.m$^{0.5}$)	Tensile Strength, σt (MPa)	Shale	0.08	0.19	0.54	4.96	0.69	0.085	0.88	19

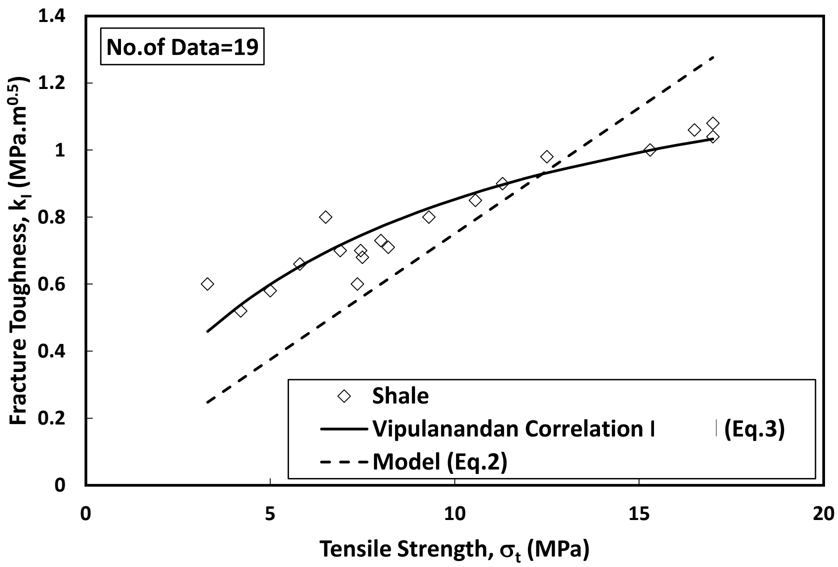

Figure 6 Correlation Between the Fracture Toughness and Tensile Strength of the Shale Rock

Failure Models (Shear Strength-Normal Stress)

Mohr-Coulomb Model

Based on Mohr-Coulomb failure model (Eq. (5)), the yield stress (τ_o), angle of internal friction (ϕ), and tensile strength (σ_t) for the shale rock were 2.7 MPa, 28^{o,} and 5.0 MPa respectively as summarized in Table 4.

Vipulanandan Model

Using 29 data collected from the literatue on the shear strength and normal stress for shale rock, Vipulanandan failure model (Eq. (3)) was used to predict the relationship. The coefficient of determination (R^2) and root mean square of error (RMSE) were 0.94 and 3.4 MPa respectively as summarized in Table 4. The yield stress (τ_o) and tensile strength (σ_t) for the shale rock were 2.6 MPa and 3.2 MPa respectively as summarized in Table 4. The Mohr-Coulomb predictions were higher than the Vipulanandan Model. The model parameters C and D for shale rock were 1.26 and 0.01 MPa^{-1} respectively as summarized in Table 4.

Maximum shear strength ($\tau_{max.}$)

Based on Eqn. 3, the Vipulanandan failure model has a limit on the maximum shear stress the rocks will tolerate. Based on the limited data, the τ_{max} for shale rock was 102 MPa as summarized in Table 4.

Table 4. Failure Model Parameters for Shale Rock

Mohr-Coulomb model (Eq.5)					Vipulanandan failure model (Eq.3)						
τ_o (MPa)	ϕ (^{o})	σ_t (MPa)	RMSE (MPa)	R^2	τ_o (MPa)	σ_t (MPa)	C	D MPa^{-1}	$\tau_{max.}$ (MPa) (Eq. 9)	RMSE (MPa)	R^2
2.7	28	5.0	3.3	0.97	2.6	3.2	1.26	0.010	102	3.4	0.94

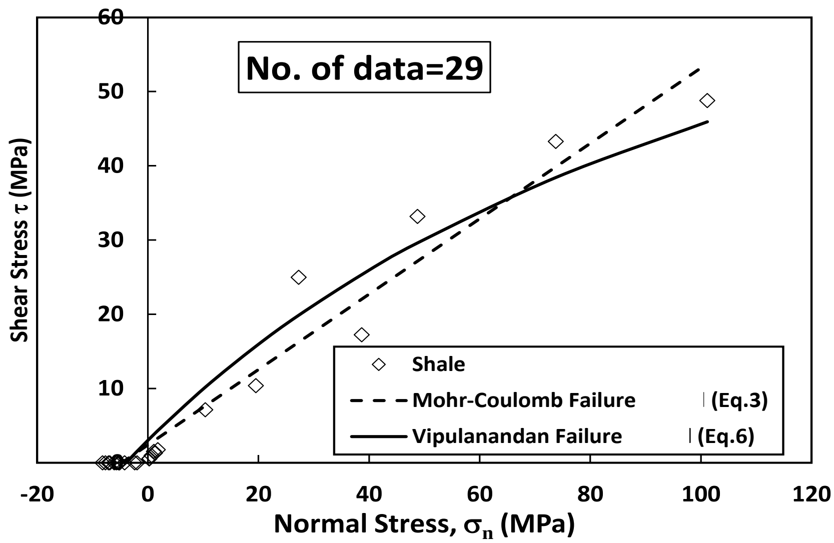

Figure 7 Comparing the Failure Model Predictions for the Shale Rock

5. CONCLUSIONS

The focus of this study was to characterize the shale rock density and strength properties based on the data collected from the literate and test performed. Correlation between tensile strength, fracture toughness and compressive strength for the shale rock was developed, based on the collected data from the literature and analytical model, the following conclusions were advanced:

1. The compressive strength (σ_c) of the shale rock varied between 2 to 200 MPa. Based on the statistical analysis the mean value of density was 2.50 gm/cm^3 respectively.
2. There were no direct correlations between the compression strength and density (γ) of the shale rock. The tensile strength to compressive strength ratio of the shale rock varied from 0.05 to 0.2 compared to 0.1 for concrete.
3. The Vipulanandan correlation model was effective in predicting the relationship between tensile strength and compressive strength of the three types of rock.
4. A new Vipulanandan failure criterion has been developed to not only better quantify the shear stress but also maximum shear strength tolerance of the rocks. The maximum shear stress ($\tau_{max.}$) for the shale rock was 102 MPa.

6. REFERENCES

1. Abdelaali, R., B. Abderrahim, B. Mohamed, G. Yves, S. Abderrahim, H. Mimoun, and S. Jamal. 2013. "Prediction of Porosity and Density of Calcarenite Rocks from P-wave Velocity Measurements." International Journal of Geosciences 4 (9). doi:10.4236/ijg.2013.49124
2. Bednarik, M., Moshammer, B., Heinrich, M., Holzer, R., Laho, M., Rabeder, J. and Unterwurzacher, M. (2014). Engineering geological properties of Leitha Limestone from historical quarries in Burgenland and Styria, Austria. Engineering geology, 176, 66-78.
3. Dott, R. H. (1996): Journal of Sedimentary Petrology, V-34, pp.623-632.
4. Karakus, M., Kumral, M., & Kilic, O. (2005). Predicting elastic properties of intact rocks from index tests using multiple regression modelling. International journal of rock mechanics and mining sciences (1997), 42(2), 323-330.

5. Mahmood, W., & Mohammed, A. (2020). New Vipulanandan pq model for particle size distribution and groutability limits for sandy soils. Journal of Testing and Evaluation, 48(5).
6. Mahmood, W., Mohammed, A., & Hama Hussein, S. (2020). Predicting mechanical properties and ultimate shear strength of gypsum, limestone and sandstone rocks using Vipulanandan models. Geomechanics and Geoengineering, 15(2), 90-106.
7. Meng, Z., and Pan, J. (2007). Correlation between petrographic characteristics and failure duration in clastic rocks. Engineering geology, 89(3), 258-265.
8. Mohammed, A. S., and Vipulanandan, C. (2014). Compressive and tensile behavior of polymer treated sulfate contaminated CL soil. Geotech. and Geolog. Engineering, 32(1), 71-83.
9. Mohammed, A. S., and Vipulanandan, C. (2014). Compressive and tensile behavior of polymer treated sulfate contaminated CL soil. Geotech. and Geolog. Engineering, 32(1), 71-83.
10. Mohammed, A., & Mahmood, W. (2018 a). Vipulanandan failure models to predict the tensile strength, compressive modulus, fracture toughness and ultimate shear strength of calcium rocks. International Journal of Geotechnical Engineering, 1-11.
11. Mohammed, A., & Mahmood, W. (2018 b). Statistical variations and new correlation models to predict the mechanical behavior and ultimate shear strength of gypsum rock. Open Engineering, 8(1), 213-226.
12. Mohammed, A., & Mahmood, W. (2019). Estimating the efficiency of the sandy soils-cement based grout interactions from particle size distribution (PSD). Geomechanics and Geoengineering, 1-18.
13. Mohammed, A., and Vipulanandan, C. (2015). Testing and modeling the short-term behavior of Lime and Fly Ash treated sulfate contaminated CL soil. Geotechnical and Geological Engineering, 33(4), 1099-1114.
14. Omar, M. (2017). Empirical correlations for predicting strength properties of rocks–United Arab Emirates. International Journal of Geotechnical Engineering, 11(3), 248-261.
15. Pettijohn, F.J. (2002): Sedimentary Rocks, Third dition, CBS ublishers and Distributors, 4596/1-A, 11 Daryaganj, New Delhi, - 110002 India, 628pp. Excavatability of Rock, Quarterly Journal of Engineering Geology, 27, pg 145-164
16. Rajabzadeh, M. A., Moosavinasab, Z., & Rakhshandehroo, G. (2012). Effects of rock classes and porosity on the relation between uniaxial compressive strength and some rock properties for carbonate rocks. Rock mechanics and rock engineering, 45(1), 113-122.
17. Sabatakakis, N., Koukis, G., Tsiambaos, G. and Papanakli, S. (2008). Index properties and strength variation controlled by microstructure for sedimentary rocks. Engineering Geology, 97(1-2), 80-90.
18. Selçuk, L., & Nar, A. (2016). Prediction of uniaxial compressive strength of intact rocks using ultrasonic pulse velocity and rebound-hammer number. Quarterly Journal of Engineering Geology and Hydrogeology, 49(1), 67-75.
19. Singh, M., Samadhiya, N. K., Kumar, A., Kumar, V. and Singh, B. (2015). A nonlinear criterion for triaxial strength of inherently anisotropic rocks. Rock Mechanics and Rock Engineering, 48(4), 1387-1405.
20. Tucker, M. E. (Ed.). (2009). Sedimentary petrology: an introduction to the origin of sedimentary rocks. John Wiley and Sons
21. Vipulanandan, C., & Mohammed, A. (2018). New Vipulanandan failure model and property correlations for sandstone, shale and limestone rocks. In IFCEE 2018 (pp. 365-376).
22. Vipulanandan, C., and Mohammed, A. S. (2014). Hyperbolic rheological model with shear stress limit for acrylamide polymer modified bentonite-drilling muds. Journal of Petroleum Science and Engineering, 122, 38-47.
23. Vipulanandan, C., Mohammed, A. and Qu, Q. (2014). Characterizing the hydraulic fracturing fluid modified with nano silica proppant. In AADE fluids technical conference and exhibition, Houston (pp. 15-16).

24. Vipulanandan, C. (2021) Smart Cement:Developing, Testing, Modeling and Real-Time Monitoring, Taylor and Francis-CRC press, London, U.K. 440 pp.
25. You, M. (2015). Strength criterion for rocks under compressive-tensile stresses and its application. Journal of Rock Mechanics and Geotechnical Engineering, 7(4), 434-439.
26. Ghafor, K., Mahmood, W., Qadir, W. and Mohammed, A. (2020 a). Effect of Particle Size Distribution of Sand on Mechanical Properties of Cement Mortar Modified with Microsilica. ACI Materials Journal, 117(1).
27. Ghafor, K., Qadir, S., Mahmood, W. and Mohammed, A. (2020 b). Statistical variations and new correlation models to predict the mechanical behaviour of the cement mortar modified with silica fume. Geomechanics and Geoengineering, 1-13.