Research Article

Study on Prediction Model of Mechanical Parameters of Rock Frozen-Thawed Damage based on NMR Technology

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In order to establish prediction models for the mechanical parameters of rock freeze-thaw damage based on nuclear magnetic resonance (NMR) technology, with reference to the laboratory test of rock mechanical parameters after freeze-thaw, combined with low-field NMR and multivariate analysis methods, PLSR and PCR prediction models for the peak stress, peak strain, and elastic modulus of frozen-thawed rocks were established. The results show that the correlation coefficient of calibration set ($R^2_{cal}$) and validation set ($R^2_{val}$) of the PLSR and PCR prediction models are both greater than 0.9, and the residual prediction deviation (RPD) of each model is greater than 3, indicating that the established prediction models have good stability, small relative error, and high prediction accuracy. The application evaluation results show that the peak stress and peak strain of frozen-thawed rocks can be accurately predicted using these models. In this paper, only the NMR tests are performed on the frozen-thawed rocks, and no rock mechanics experiments are performed. The research results provide a new method for the research of rock freeze-thaw damage.

1. Introduction

In geotechnical engineering in cold areas, frozen-thawed cycle is one of the factors affecting the deterioration of rock mechanical properties [1, 2]. Under the action of repeated frozen-thawed cycles, the quality of rock mass will be damaged and degraded, resulting in strength decline, easily causing frozen-thawed disasters such as frozen-thawed denudation and rock slope landslide, which has a significant impact on the stability of rock mass engineering in cold regions [3]. Therefore, studying and mastering the variation law of macroscopic mechanical parameters of rock under freezing and thawing can provide theoretical basis for the prevention and control of freezing and thawing disasters of rock mass engineering in cold areas.

Nuclear magnetic resonance (NMR) technology has been widely used in the field of mesostructural damage detection of porous media materials such as rocks and soil. In the mechanical study of frozen-thawed rock by NMR technology, the research method combining macro- and micro- is usually adopted. The microstructure test is to obtain CPMG spin echo attenuation, curved through NMR technology, and then get $T_2$ spectrum curve after inversion. Then, parameters such as porosity, pore size distribution, and pore fractal dimension of rock blocks are obtained through various algorithms around $T_2$ spectrum [4, 5], so as to master pore distribution and crack development characteristics inside rock under frozen-thawed cycles. In terms of macroscopic mechanics, mechanical test experiments of frozen-thawed rocks were carried out to obtain the physical and mechanical parameters of rocks under frozen-thawed cycles and study the mechanical behavior laws of rocks under frozen-thawed cycles [6, 7]. Finally, combined with the theories of damage mechanics, fracture mechanics, and the principle of NMR, the influence law of crack space characteristics, initial damage, and frozen-thawed action on rock damage was analyzed, the relationship between crack space characteristics and macroscopic mechanical parameters was found out, and a rock damage model considering frozen-thawed effect was established. For example, Zhou et al. [8] conducted NMR and impact loading tests on sandstone under different frozen-thawed cycles and concluded that the relationship between porosity and dynamic peak strength was polynomial. Ma et al. [9] carried out SHPB...
dynamic compression tests on soft rock and sandy mudstone that experienced different frozen-thawed cycles, and the results showed that the uniaxial dynamic compressive strength of both rock samples showed a logarithmic decreasing trend with the increase of frozen-thawed cycles. This research method and idea provide a good foundation for promoting the application of NMR technology in the study of rock frozen-thawed damage, but there are also some shortcomings such as long experimental period, high cost, and inability to realize real-time online testing.

In order to save test time and cost, a large number of scholars focused on the establishment of rock damage prediction model. Deng et al. [10] used the fractal dimension of macropores as independent variable to perform linear fitting of compressive strength, macropore volume, and fractal dimension of macropore diameter, respectively, deduced the specific expression of the strength model, and established a strength prediction model for sandstone-like materials. Xiong et al. [11] used genetic algorithm (GA) and artificial neural network (ANN) method to establish a database of rock triaxial compressive strength, including four model inputs and one output of p-wave velocity, porosity, confining pressure, and frozen-thawed cycles. Based on genetic algorithm, the structure, initial connection weight, and deviation of neural network were gradually optimized. The mixed GA-ANN model was obtained to predict the triaxial compressive strength of sandstone under different frozen-thawed conditions. Huang et al. [12] established an exponential attenuation model of uniaxial compressive strength of frozen-thawed sandstone by taking the initial porosity, elastic modulus, and tensile strength of sandstone as the initial parameters, which can estimate the loss of uniaxial compressive strength of sandstone after different frozen-thawed cycles without mechanical and frozen-thawed tests. At present, most of the existing achievements were based on porosity, fractal dimension, and other parameters as independent variables to construct prediction models, and these parameters are obtained by mathematical methods such as inversion algorithm and data fitting, which often have certain theoretical errors with the original test data. Behnia et al. [13] used the gene expression programming (GEP) method to predict the uniaxial compressive strength (UCS) and static elastic modulus (E) of intact rocks from their quartz content, dry density, and porosity. In the study of Fang et al. [14], porosity (n), Schmidt hammer rebound number (R), p-wave velocity (Vp), and point load strength index (Is(50)) were selected as input parameters; four models were proposed to evaluate the strength properties of granite block samples (UCS), including artificial neural network (ANN), hybrid artificial neural network with imperialist competition algorithm (ICA-ANN), hybrid artificial neural network with artificial bee colony (ABC-ANN), and genetic programming (GP) method. The results showed that GP model has the best performance, and the uniaxial compressive strength of granite samples can be estimated accurately.

From the above studies, it can be found that many intelligent algorithms were used to predict rock mechanical properties. But the input parameters of the model are mostly rock characteristic parameters, for example, the porosity of rocks. There are few related research reports on the prediction of rock mechanical parameters directly using the original decay curve of NMR as the model input parameter. In fact, the research methods and ideas have been widely used in the field of food nondestructive testing. Based on CPMG data, Zang et al. [15] have established a prediction model of water and fat content of small yellow croaker to quickly identify adulterated small yellow croaker. Wang et al. [16] combining with low-field NMR data and multivariate analysis method have identified adulterated olive oil quickly. The above research provides a reference for the establishment of damage prediction model of macroscopic mechanical parameters of frozen-thawed rocks.

In this study, using the results of NMR test and mechanical test as reference values, fast prediction models of peak stress, peak strain, and elastic modulus of frozen-thawed rocks based on LF-NMR technology were established to achieve rapid and nondestructive analysis of macromechanical parameters of frozen-thawed rocks under the condition of NMR test only.

2. Data Acquisition

2.1. CPMG Spin Echo Signal Attenuation Data. In NMR detection of rock, CPMG pulse train can generate a series of spin echoes, which constitute the original NMR data. The attenuation of the spin echo string is a function of the number and distribution of hydrogen nuclei in the fluid, and its initial amplitude is related to the number of hydrogen nuclei in the fluid within the detection range. The echo amplitude decreases with the increase of time, presenting an exponential attenuation feature [17]. Therefore, the attenuation data of spin echo string can be converted into T2 spectrum curve through inversion, so as to obtain porosity, pore size distribution, T2 cut-off value, permeability, and other important parameters. Research results have proved that there is a functional relationship between microscopic parameters such as porosity and macroscopic mechanical parameters of rock samples [18, 19]. As the original attenuation curve of NMR test, there must be some relationship between CPMG spin echo signal attenuation data and macroscopic mechanical parameters of rock. Therefore, multivariate analysis method can be used to find the relationship between CPMG spin echo signal attenuation data and mechanical parameters of frozen-thawed rock, so as to establish a prediction model of mechanical parameters of frozen-thawed rock based on NMR parameters.

According to the requirements of multivariable analysis method, the number of CPMG spin echo signal attenuation data involved in model building should be the same, and the test duration of each data point should be similar. Namely, the start time and end time of measurement should be consistent or similar; otherwise, multivariable analysis cannot be carried out. By analyzing the CPMG sequence of basic parameters on the measuring time and the influence of the acquisition data points, it was found that the sampling frequency, echo time, and number three parameters affect the spin echo signal attenuation curve test of the initial value and end value of time, and cumulative frequency affects
the number of data points collected, so when choosing the NMR test data of the rock, rock sample data with the same or similar parameters should be selected as far as possible.

2.2. Rock Mechanics Parameters. According to the selection requirements of rock NMR test data, NMR spin echo attenuation data of 15 yellow sandstones subjected to freezing and thawing and their corresponding peak stress, peak strain, and elastic modulus are selected. The number of frozen-thawed cycles, mechanical experiment types, and macromechanical parameter measurement values is shown in Table 1.

3. Macromechanical Prediction Model of Frozen-Thawed Rock

3.1. Establishment of Model. The correlation model was established by using LF-NMR test data and mechanical test results. Twelve rock samples with serial numbers 1, 3-4, 6-12, and 13-15 were selected to establish the prediction model, and three rock samples with serial numbers 2, 5, and 13 were used to verify the accuracy of the model. The model building process is as follows:

1. A prediction model was established as the first step. All CPMG spin echo signal attenuation data of each rock sample, namely, 200 CPMG data points, as well as the results of mechanical parameters including peak stress, peak strain, and elastic modulus, were listed in a $12 \times 203$ matrix, and the baseline adjustment was performed on the data in advance.

2. Taking the mechanical test results as reference values, the matrix of independent variables was the attenuation amplitude of spin echo signal ($X$), and each row of data matrix $X$ gave the attenuation amplitude of spin echo signal of a frozen-thawed rock sample. The dependent variable was the corresponding macromechanical parameter ($Y$).

3. Using multivariate analysis software, PLSR prediction model and PCR prediction model of peak stress, peak strain, and elastic modulus were established, respectively.

4. The established PLSR and PCR prediction models were applied to predict the mechanical parameters of the rock samples to be tested, and the predicted values of peak stress, peak strain, and elastic modulus of the frozen-thawed rock samples were obtained.

5. The peak stress, peak strain, and elastic modulus of frozen-thawed rock samples obtained from mechanical tests were compared and verified.

3.2. Model Inspection. The model can be tested from three aspects: correlation, prediction ability, and accuracy of prediction results [15]. The correlation coefficient of the model can be used to evaluate the accuracy and stability of the model. When the correlation coefficient of calibration set and validation set ($R^2_{cal}$ and $R^2_{val}$) is closer to 1, the better the correlation of the model is. The calculation formula of correlation coefficient is shown in Formula (1). Generally, when $R^2 > 0.9$, it can be considered that the model has good correlation.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2},$$

where $\hat{y}_i$ is the macroscopic mechanical parameters obtained by regression of NMR data, $y_i$ is the macroscopic mechanical parameters of rock samples obtained by mechanical experiments, $\bar{y}$ is the average value of macroscopic mechanical parameters of rock samples obtained by mechanical experiments, and $n$ is the number of sample sets.

Figures 1–3 are the correlation diagrams of the predicted values and measured values of PLSR and PCR prediction models for peak stress, peak strain, and elastic modulus of frozen-thawed rocks, respectively. By observing the scattered distribution diagrams of the calibration set and verification set of peak stress, peak strain, and elastic modulus of frozen-thawed rocks, it can be found that the data points are evenly distributed on both sides of the tropic of cancer, and the correlation coefficients of the calibration set and verification set are both greater than 0.9, which indicates that the established prediction models have good correlation. In addition, the data points in the figure are concentrated in the lower left corner and the upper right corner. The reason may be that the original data used to establish the model are obtained by uniaxial compression and impact loading mechanical experiments of yellow sandstone, respectively. The peak stress, peak strain, and elastic modulus of different mechanical loading methods are quite different, which leads to the big difference between the data of correction set and verification set. After the equation regression, the linear regression equations of each model are obtained (as shown in Figure 1): $Y = AX + B$, where $X$ is the measured value of peak stress, peak strain, and elastic modulus of frozen-thawed rock and $Y$ is the predicted value of mechanical parameters of frozen-thawed rock.

In terms of model prediction ability, the root mean square error (RMSEC and RMSEV) of calibration set and verification set can reflect the model’s prediction ability. The root mean square error can be obtained by Formula (2). The smaller the value is, the better the model’s prediction ability is. In terms of accuracy of prediction results, residual prediction deviation (RPD) can be evaluated. The residual prediction deviation can be obtained by Formula (3), where $SD$ is standard deviation, $RPD > 3$, and $R^2 \geq 0.9$, indicating good prediction results and high reliability.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2},$$

$$RPD = \frac{SD}{RMSEV}.$$
in this paper are obtained, as shown in Table 2. As can be seen from Table 2, RMSEC and RMSEV of peak stress PLSR model are 2.693 and 3.085, respectively, and RMSEC and RMSEV of PCR model are 2.695 and 3.086, respectively. There is little difference in root mean square error of the two models, and both values are large, indicating that the prediction ability of peak stress of the two models is weak. The RMSEC and RMSEV of PLSR model of elastic modulus are 0.209 and 0.439, respectively, and the RMSEC and RMSEV of PCR model are 0.266 and 0.451, respectively. The difference of root mean square error of the two models is small and the value is low, indicating that the prediction ability of elastic modulus of the two models is good. The RMSEC and RMSEV of the PLSR model and the PCR model for peak strain are 0.028 and 0.033, respectively. The root mean square error of the two models is the same and the lowest compared with the first two models, indicating that the two models have the strongest ability to predict peak strain. In addition, the six prediction models all satisfy $R^2 > 0.9$ and RPD > 3, indicating that the established model has high reliability in predicting results.

### Table 1: Physical and mechanical parameters of surface rock samples.

| Serial number | Frozen-thawed times/times | Mechanical experiment | Peak stress (MPa) | Peak strain (%) | Elastic modulus (GPa) |
|---------------|---------------------------|-----------------------|------------------|-----------------|----------------------|
| 1             | 60                        | Uniaxial compression  | 61.2             | 0.95            | 12.4                 |
| 2             | 60                        | Uniaxial compression  | 59.3             | 0.97            | 13.1                 |
| 3             | 60                        | Uniaxial compression  | 56.4             | 0.94            | 12.3                 |
| 4             | 60                        | Shock loading         | 84.2             | 0.69            | 9.25                 |
| 5             | 60                        | Shock loading         | 84.9             | 0.69            | 9.56                 |
| 6             | 60                        | Shock loading         | 80.7             | 0.68            | 9.05                 |
| 7             | 60                        | Shock loading         | 85.4             | 0.68            | 9.18                 |
| 8             | 60                        | Shock loading         | 83.1             | 0.69            | 9.24                 |
| 9             | 100                       | Uniaxial compression  | 55.4             | 1.01            | 11.6                 |
| 10            | 100                       | Uniaxial compression  | 54.9             | 0.97            | 11.2                 |
| 11            | 100                       | Shock loading         | 79.2             | 0.71            | 8.34                 |
| 12            | 100                       | Shock loading         | 74.3             | 0.7             | 8.31                 |
| 13            | 100                       | Shock loading         | 80.4             | 0.7             | 8.23                 |
| 14            | 100                       | Shock loading         | 82.4             | 0.69            | 8.84                 |
| 15            | 100                       | Shock loading         | 75.4             | 0.78            | 8.21                 |

3.3. Application Evaluation of the Model. Three rock samples with serial numbers 2, 5, and 13 in Table 1 were used to verify the accuracy of the prediction model. The measured values of mechanical experiments and the elastic modulus, peak stress, and peak strain of frozen-thawed rock obtained by PLSR and PCR prediction models are listed in Table 3. The results showed that the relative errors between the elastic modulus obtained by PLSR and
PCR models and the elastic modulus obtained by mechanical test are 2.80%-7.56% and 4.16%-8.31%, respectively, indicating that the PLSR model is more accurate than the PCR model. The relative errors of the peak stress obtained by PLSR and PCR models and the peak stress obtained by mechanical test are in the range of 0.71%~4.09%, and the accuracy of the two models is the same, with small relative errors and high accuracy. The relative errors of peak strain obtained by PLSR and PCR prediction models and peak strain obtained by mechanical test are between 0.61% and 2.04%. The accuracy of peak strain prediction by PLSR and PCR prediction model is the same, and the relative errors are the lowest and the accuracy is the highest. In conclusion, among the three mechanical parameters, the PLSR and PCR

| Model | Mechanical parameters | RMSEC (%) | RMSEV (%) | RPD |
|-------|-----------------------|-----------|-----------|-----|
| PLSR  | Peak stress           | 2.693     | 3.085     | 10.150 |
|       | Peak strain           | 0.028     | 0.033     | 1129.735 |
|       | Modulus of elasticity | 0.209     | 0.439     | 608.836 |
| PCR   | Peak stress           | 2.695     | 3.086     | 86.694 |
|       | Peak strain           | 0.028     | 0.033     | 84.533 |
|       | Modulus of elasticity | 0.266     | 0.451     | 6.122 |

PCR models and the elastic modulus obtained by mechanical test are 2.80%-7.56% and 4.16%-8.31%, respectively, indicating that the PLSR model is more accurate than the PCR model. The relative errors of the peak stress obtained by PLSR and PCR models and the peak stress obtained by mechanical test are in the range of 0.71%-4.09%, and the accuracy of the two models is the same, with small relative errors and high accuracy. The relative errors of peak strain obtained by PLSR and PCR prediction models and peak strain obtained by mechanical test are between 0.61% and 2.04%. The accuracy of peak strain prediction by PLSR and PCR prediction model is the same, and the relative errors are the lowest and the accuracy is the highest. In conclusion, among the three mechanical parameters, the PLSR and PCR
Table 3: Comparison of mechanical parameters between PLSR and PCR prediction models and mechanical experiments.

| Mode | Serial number | Elastic modulus (GPa) | Relative error (%) | Peak stress (MPa) | Relative error (%) | Peak strain (%) | Relative error |
|------|---------------|-----------------------|--------------------|-------------------|--------------------|----------------|---------------|
|      |               | P                     | M                  | P                 | M                  | P              | M             |
| PLSR | 1             | 12.11                 | 13.10              | 7.56              | 58.35              | 59.30          | 1.61          | 0.95          | 0.97          | 2.04%         |
|      | 2             | 9.29                  | 9.56               | 2.80              | 81.43              | 84.90          | 4.09          | 0.69          | 0.69          | 0.61%         |
|      | 3             | 8.50                  | 8.23               | 3.24              | 79.88              | 80.40          | 0.65          | 0.71          | 0.70          | 1.63%         |
| PCR  | 1             | 12.01                 | 13.10              | 8.31              | 58.34              | 59.30          | 1.61          | 0.95          | 0.97          | 2.04%         |
|      | 2             | 8.89                  | 9.56               | 7.04              | 81.43              | 84.90          | 4.09          | 0.69          | 0.69          | 0.61%         |
|      | 3             | 8.57                  | 8.23               | 4.16              | 79.88              | 80.40          | 0.65          | 0.71          | 0.70          | 1.63%         |

Note: P: predict; M: measure.
models of peak strain have the highest accuracy, followed by the PLSR and PCR models of peak stress, and the PCR model of elastic modulus has the worst accuracy.

4. Discussion

As known, rock is a heterogeneous anisotropic material. The porosity, pore distribution, and internal particle bonding of different rock samples are also different. The freeze-thawed damage mechanism of rock can be stated as follows: on the one hand, the water in the internal fractures of the rock freezes and expands under the action of low temperature, which causes the development and expanding of the internal pores. On the other hand, the frozen ice dissolves into water under the action of high temperature and then migrates between the pores. This can lead to accelerated penetration of the internal fractures of the rock, thereby deteriorating the mechanical properties. It can be seen that under different freeze-thawed cycles and under different initial damage of rock, the macroscopic mechanical parameters of rock are more discrete. Therefore, when establishing a prediction model, it should be ensured that the selected rock samples have the same lithology, similar primary pores, and appearance integrity.

Moreover, for better multivariable analysis, CPMG spin echo signal attenuation data of rock samples involved in modeling should be the same in number, and their measurement start time and end time should be consistent or close. Therefore, the sampling frequency, echo time, echo number, and accumulation times should be set the same or similar in NMR test.

It is worth noting that not only the number of freeze-thawed cycles and porosity but also rock type, joint fracture development, and loading rate are also influencing factors of rock mechanical parameters. In the next research, more parameters should be introduced for comprehensive analysis. In addition, the accuracy of the prediction model is related to the number of samples. Generally speaking, the more samples, the higher the accuracy of the model. Therefore, more data should be collected to optimize the model in the next research.

5. Conclusion

In this paper, a fast prediction method for macroscopic mechanical parameters of frozen-thawed rock was established based on LF-NMR technology. Combined with the spin echo attenuation data obtained by CPMG sequence and multivariate analysis method, PLSR and PCR methods were, respectively, used to establish the prediction model of peak stress, peak strain, and elastic modulus of frozen-thawed rock, and the following conclusions were obtained.

(1) Among the 6 models established, the correlation coefficients are all greater than 0.9 and the correlation is good. The PLSR and PCR models had the best prediction ability of peak strain, and the RMSEC and RMSEV of the two models were consistent, which were 0.028 and 0.033, respectively. The worst are the PLSR and PCR models for peak stress. The PPD of the six models were all greater than 3, which met the requirements in terms of accuracy of prediction results.

(2) It has been verified that the PLSR and PCR models of peak strain have the highest accuracy, followed by the PLSR and PCR models of peak stress, and the PCR model of elastic modulus has the worst accuracy. The relative errors of PLSR and PCR prediction models for elastic modulus, peak stress, and peak strain are 2.80%–8.31%, 0.71%–4.09%, and 0.61%–2.04%, respectively. Namely, the peak stress and peak strain of frozen-thawed rocks can be accurately predicted using these models.

Data Availability

The data can be found in the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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