Research Article

The Influence of Physical and Chemical Reactions on Water Leakage in a Multiarch Tunnel

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Abstract

In many tunnels in China, the groundwater is acidic and carbonated, causing challenges in the prevention and control of leakages of existing tunnels and tunnels under construction. Research on tunnel leakage and the physical and chemical effects of water due to water-rock interactions is a trending topic. In addition, there is a big difference between the waterproof and drainage of multiarch tunnels and separate tunnels. In this study, the mechanism of the interaction between the groundwater and the surrounding rock of a multiarch tunnel were analyzed. The relationship between the leakage of a multiarch tunnel and the interaction between the surrounding rocks and groundwater was determined by analyzing the interaction between the chemical components in the groundwater, rocks, and the concrete lining. A mathematical model was established based on the physical and chemical reactions in the rock surrounding the tunnel, and the RNCDX.FOR program was compiled using the simplex Monte Carlo method. The total free energy in the entire system varied significantly, and the value of objective function \( J \) reflected the trend of the system’s spontaneous reaction. As \( J \) decreased, the reaction power of the system increased. The more significant the erosion of the rocks was by the groundwater, the more channels were created by the groundwater in the rock, and the more likely the water leakage was.

1. Introduction

Water-rock interaction research is one of the leading topics in mechanics and earth sciences. The interaction is referred to as "solid-fluid coupling" in mechanics and "water-rock interaction" in earth sciences. The focus of the former research is on the fundamental laws of mechanical coupling between solids and fluids; the latter is concentrated on the laws of the physicochemical reactions and the physical and chemical characteristics of the rocks and water under high-temperature high-pressure conditions. As an interdisciplinary discipline that integrates civil engineering and geology, geotechnical engineering has focused on rock body hydraulics, i.e., a study of the laws from the perspective of the interaction of the seepage field and stress field. Hellevang et al. [1] provided a guide to model kinetically constrained \( \text{CO}_2 \)-water-rock interactions. Kaszuba et al. [2] demonstrated that the interaction between \( \text{CO}_2 \), water, and rock could lead to the massive dissolution and precipitation of minerals, and numerous techniques existed for obtaining experimental data. Zhao et al. [3] used the discrete element method to analyze the effect of water-rock mechanical interaction and the combination of physical and chemical effects on the deformation of a reservoir bank slope. Recently, the chemical interaction between water and rocks has been increasingly investigated [4–8], especially in the construction of tunnels in China, where the groundwater is acidic and carbonated. These conditions have caused significant challenges in the prevention and control of leakages of existing tunnels and tunnels under construction, as shown in Figure 1. Wang et al. [9] analyzed the mineral origin of carbonate cement, the mechanism of precipitation, the
evolution and distribution of pore fluids, and the interaction between water and rock and its impact on reservoir quality. At present, there are few random physical and chemical simulation studies on water leakage caused by water-rock interaction in tunnels.

In terms of physical chemistry, the main elements that exhibit chemical reactions in geotechnical engineering include the groundwater and its chemical components, rock formations, organic matter, and materials used in engineering, such as concrete. These elements will interact under certain temperature, pressure, and concentration conditions, produce energy exchange, and generate energy output using input from the environment [10–14]. In addition, the external environment promotes or prevents interactions. Zheng and Liu [5] first used physical and chemical simulations to analyze an aquifer in the surrounding rock of a tunnel, and the model was an optimized linear model. Wang et al. [15] analyzed the mechanism of water-rock interaction inside the aquifer. Many Chinese scholars have investigated the water-rock interaction [16–19]. However, these studies had two limitations. First, most studies used linear programming models, and nonlinearity has not been analyzed in detail. Second, insufficient sample data were used. Most studies did not use sample data from multiple trials, but only from a single trial. The sample data were averaged, and the average value was used for analysis and calculation. Therefore, the mutual influence of the system inside and outside the surrounding rock of the multiarch tunnel and the random changes were ignored, which produced simulation results that did not represent actual conditions.

In this study, the internal energy of the surrounding rock of the tunnel is simulated to determine the degree of erosion and the connectivity of the surrounding rock.

There is a big difference between the waterproof and drainage of multiarch tunnels and separate tunnels. Mao et al. [20, 21] used 3D numerical simulation to analyze the water leakage susceptible area of the loess multiarch tunnel. The results show that the water disaster susceptible areas for loess multiarch tunnels during the construction period mainly concentrated in the midpartition, arch springs of the left and right tunnels, and the tunnel face. In this study, the prevention and control of water leakage in a multiarch tunnel is mainly discussed from the perspective of the interaction mechanism between groundwater and surrounding rock.

A mathematical programming model of the physical-chemical conditions of the rock is established. In other words, the chemical reaction inside the surrounding rock of the multiarch tunnel is used as the objective function, and the equilibrium principle, mass conservation law, charge conservation law, and other conditions are used as constraints of the model. After obtaining a model solution, the water-rock interaction inside the surrounding rock of the multiarch tunnel is analyzed to determine the degree of erosion of the surrounding rock caused by the groundwater.

The use of random numbers in the Monte Carlo analysis ensures that the data provide a realistic simulation of actual conditions to reflect the mechanism of water-rock interaction in the surrounding rock of multiarch tunnels. The analysis of the internal chemical reaction of the surrounding rock can provide a theoretical basis for the waterproofing, drainage design, and construction of multiarch tunnels and the prevention and treatment of water leakage.

2. Mathematical Model of Water-Rock Interaction

2.1. Mathematical Model. The water-rock interaction can be regarded as an organic connection or a large system of mutual influence [22–25]. In a system with certain pressure, temperature, and concentration conditions, the chemical reaction always proceeds in the direction where the free energy becomes smaller and tends to balance. According to the principle of thermodynamics, the smaller the value of $\Delta G_f$, the stronger the positive reaction trend. Accordingly, take the minimum sum of the free energy changes of each physical and chemical reaction in the groundwater system as the objective function. The constraint conditions are established based on the laws of the conservation of mass, conservation of charge, and neutrality among the chemical components in the groundwater system. The objective
2.2. Random Number Generation

The mathematical model:

\[
P = \min X = \sum_{i=1}^{n} \Delta G_{fi} X_i, \\
\sum_{i=1}^{n} a_{ij} X_i = d_j, \quad (j = 1, 2, \ldots, m), \\
X_i > 0,
\]

where \( P \) is the free energy change of reaction in the system, \( X_i \) is the amount of the \( i \)-th physicochemical reaction, \( \text{mmol/L} \). If \( X_i > 0 \), there is a positive reaction inside the system; if \( X_i < 0 \), there is a reverse reaction inside the system; if \( X_i = 0 \), the system is in equilibrium. \( \Delta G_{fi} \) is the free energy change of the \( i \)-th chemical reaction, \( \text{J:mmol}^{-1} \). \( a_{ij} \) is the stoichiometric number of the \( k \)-th component in the corresponding mineral of the \( i \)-th physicochemical reaction, and \( \beta_l \) is the stoichiometric number of the \( k \)-th component in the corresponding mineral of the generated phase; \( d_j \) is the concentration difference between the dissolution solution and the initial solution in the \( j \)-th component; \( j = 1, 2, \ldots, m \), and \( m \) is the number of equations with constraint conditions. This mathematical model is of universal significance for describing complex systems of water-rock interactions [25].

2.2.2. The Monte Carlo Stochastic Simulation Using the Simplex Method

The Monte Carlo method or random simulation method is based on random numbers. The Monte Carlo method was developed in the 1940s. As early as the 17th century, people knew that the probability of an event was determined by the frequency of the event. In the 19th century, people used a needle throwing test to determine \( \pi \). The emergence of electronic computers in the 1940s and the subsequent development of high-speed electronic computers in recent years have made it possible to simulate extensive experiments and rapidly perform mathematical calculations. For example, consider a square with a side length of 1 on a plane and an irregularly shaped figure inside; the problem is to find the area of the irregular figure. The Monte Carlo method uses randomization to solve this problem. \( N \) points are randomly created in the square, and \( M \) points fall within the figure; the area of the figure is approximately \( (M/N) \). The Monte Carlo method can be used to deal with the "curse of dimensionality," because the computational complexity of this method does not depend on the dimensionality. Problems that were previously impossible to solve can be solved using the Monte Carlo method. Scientists have proposed many so-called "variance reduction" techniques to increase the efficiency of the method. The Monte Carlo method differs considerably from general calculation methods. The latter is not well suited to solve problems with multiple dimensions or complex factors, whereas the Monte Carlo method is appropriate for such problems. Therefore, the Monte Carlo method
has been rapidly developed since it was developed and has become an indispensable and important part of computational mathematics.

Each \( b_j \) in the Monte Carlo system is a random variable. According to the linear programming model, the internal \( b_j \) implementation is always true. In this way, we randomly extract \( [b'_1, b'_2, \ldots, b'_N] \) corresponding to \( b_j \) from the random numbers and use the simplex method to find a set of solutions to \( X'_j = [x'_1, x'_2, \ldots, x'_N] \) using equation (1). By analogy, this step is repeated to produce \( N \) sets of solutions until \( N \) tends to infinity. When all the physical quantities in the system have been described, the characteristics of the physical quantities in the system and the distribution are obtained.

Equation (6) is the definition of the mean value and equation (7) is the definition of the standard deviation:

\[
\mu = \frac{1}{N} \sum_{i=1}^{N} X_i, \quad (6)
\]

\[
\sigma = \left[ \frac{1}{N-1} \sum_{i=1}^{N} (X_i - \mu)^2 \right]^{1/2}. \quad (7)
\]

The Monte Carlo method is implemented and a program is written (RNDDX.FOR) for use in the subsequent case study.

3. Case Study

3.1. Hydrogeological and Topographic Features in the Tunnel Site Area. The exit of the multiarch tunnel is located on the east side of the downslope of low- and midelevation mountains. The slope is covered with gravel and soil layers and consists of strongly-weekly weathered marl and limestone. The gravel soil layer has a maximum thickness of 2.80 m, the thickness of the strongly weathered marl is 1.10–9.20 m, and the exposed thickness of the weakly weathered marl and limestone is 22.94–37.38 m. The natural slope of the hillside is 30–40°, the azimuth angle of the free slope of the hillside is 162°, and the slope oblique to the course is about 75°. The occurrence of bedrock is 5°–30°, and the gravel soil cover at the entrance is thin (0.60–2.80 m). The weathered fissures of the underlying bedrock are well developed, and the rock mass is highly fragmented, showing a fragmented-fissured block structure with poor integrity. The vertical slope velocity of the surrounding rock is \( V_p = 380–1800 \text{ m/s} \), and the surrounding rock is classified as grade V. The conditions for the formation of caves are poor, and the surrounding rock prone to collapse.

The gravel soil is above the groundwater level and has strong water permeability. Karst water occurs about 500 m from the cave entrance, and the water volume is large. Due to a large amount of water during the construction, grouting was used as an antiseepage curtain to facilitate construction. However, after one year of operation of the tunnel, significant water leakage occurred, especially at a distance of 500 m from the entrance of the tunnel. The field data indicated that the pH value at a distance of 1000 m from the cave entrance was low, and the water had high concentrations of dissolved CO2. The bedrock is quartz sandstone containing 10% shale, and the dominant minerals are mica, quartz, a small amount of pyrophyllite, kaolinite, and montmorillonite. Part of the bedrock is carbon shale, with an organic matter content of 4% to 8% [26, 27]. The rocks are highly broken. Due to the long-term immersion in the groundwater and resulting corrosion, some rocks have softened. The field investigation also found that the groundwater had eroded the antiseepage curtain due to cement hydrates in the groundwater, indicating that the chemical components in the groundwater and rock had interacted with the concrete.

Under certain conditions, the water-rock interaction in the area surrounding the tunnel can cause different materials in the surrounding rock to undergo chemical reactions, as shown in Table 1. The physicochemical reactions in the system are mutually reinforcing, and one reaction will promote another reaction, thus forming a reaction chain of the entire system. Over time, the physicochemical reactions continue, and a groundwater channel is formed and is being continuously connected and unblocked, increasing the water leakage in the tunnel. Depending on the interaction between the components in the surrounding rock, the groundwater components, the organic substances, the components of the concrete grouting curtain, the free energy produced by the reactants and products during the processes determine the reactant's standard free energy change (\( \Delta G_j \)).

The monitoring data of the groundwater and surrounding rock in the tunnel and the drainage holes created during construction indicate that the groundwater behind the grouting curtain is the dominant source of recharge. Thus, the groundwater is the initial liquid in the tunnel area, and the discharge liquid of the drainage holes is the dissolution liquid. The chemical composition and the differences between the initial liquid and the dissolution liquid are shown in Table 2. Both variables follow a normal distribution. The difference between the two can be expressed by statistical parameters. The mean of the difference equals the mean of the dissolution solution minus the mean value of the initial solution. The variance of the difference is the square root of the sum of squares of the variance of the dissolution solution and the initial solution; it follows a normal distribution. Four drainage holes are selected as examples for the analysis, namely hole 1, hole 2, hole 3, and hole 4 (Table 2).

3.2. The Establishment of the Mathematical Model. According to the physicochemical reactions and the free energy changes (Table 1) and the random samples of the difference between the initial solution and the dissolution solution of the components in Table 2, the following model is established:
In the processing of random numbers, some random numbers may not conform to the principles of equilibrium, the conservation of mass, the conservation of charge, and the principle of minimum energy, resulting in a mathematical model with no solution. In the calculation analysis, these random numbers are removed, and the Monte Carlo principle is used to obtain the characteristic value of the reaction amount of each water-rock interaction.

3.3. Mathematical Model Solution. Studies have shown that the number of simulations is crucial in the simulation of Monte Carlo random numbers and affects not only the rationality of the simulation results but also the accuracy of the simulation. Therefore, we tested different numbers of simulations and considered the calculation time and other factors. Ultimately, 1000 simulations were deemed reasonable and met the accuracy requirements. The results of the random simulation of the state of the water-rock interaction system are shown in Table 3.

4. Results and Discussion

The results show that the reaction amounts $X_1 \sim X_2$ in Table 3 are zero, indicating that the reaction of albite and calcite did not occur, i.e., $NaAlSi_3O_8 + CO_2 + 5.5H_2O \rightarrow 0.5NaAlSi_3(OH)_4 + Na^+ + 2H_2SiO_4 + HCO_3^-$, $CaCO_3 + CO_2 + H_2O \rightarrow Ca^2+ + 2HCO_3^-$. However, this is not the case. The model of the water-rock interaction does not reflect this type of chemical reaction process but only reflects the direction of the chemical reaction of the entire water-rock
The numbers 3, 4, 5, 6, 7, 8, 9, and 10 in Table 1 indicate that the main components involved in the reaction are Ca (OH)$_2$, organic matter, CO$_2$, and HCO$_3^-$.
Therefore, dynamic water-rock interaction occurred about 1000 m from the opening of the cave. The variance value was also relatively large, indicating the occurrence of a spontaneous reaction in the system. As a result, the connectivity of the surrounding rock of the multiarch tunnel was increased, resulting in continuous leakage.

### Notations

- \( P \): Free energy change of reaction in the system
- \( X_i \): Amount of the \( i \)-th physicochemical reaction
- \( a_{ij} \): Stoichiometric coefficient of the \( j \)-th element in the \( i \)-th physical and chemical reaction mineral
- \( d_j \): Concentration difference between the dissolution solution and the initial solution in the \( j \)-th component
- \( m \): Number of equations with constraint conditions
- \( x \): Random variable
- \( l, w \): Upper and lower limits of the distribution of the random variable
- \( u \): Mean
- \( \sigma^2 \): Variance
- \( b_j \): Constant
- \( \sigma \): Standard deviation
- \( J \): Objective function value
- \( X_1 \sim X_{10} \): Number of millimoles of reactants participating in the reaction per liter of groundwater.

### Data Availability

The data used in the study are available upon request to the corresponding author.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

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