Numerical Simulation and Effect Analysis of Hydrogen Sulfide Treatment by Advanced Alkali Injection in Tunnel Face of Highway Tunnel

Erkang Li*[a], Jihua Wang[a], Jiayao Li[a], Luying Hao[b]

[a] School of Energy Science and Engineering, Henan Polytechnic University, Jiaozuo, Henan, 454000, China;
[b] School of Tourism, Henan Normal University, Xinxiang, Henan, 453007, China

*Email: 212302020091@home.hpu.edu.cn

Abstract. H_2S gas overflow during tunnel excavation and operation will endanger workers and damage mechanical equipment. The injection of alkali into the tunnel face can significantly reduce the tunnel H_2S emission. Using the chemical reaction module in COMSOL Multiphysics software, combined with the occurrence characteristics of H_2S in tunnel rock mass and the parameters of alkali injection, the numerical simulation of H_2S treatment by $NaHCO_3$ injection in rock mass was carried out, and the diffusion law of alkali solution in rock mass and the effect of H_2S treatment were analyzed. The results show that the content of H_2S in the rock mass area of alkali infiltration is obviously reduced, and the influence range of alkali injection increases with the extension of alkali injection time. After 32 hours of continuous alkali injection, H_2S in the rock mass is almost completely neutralized within 10 m from the hole. There is a significant difference between the effect of double-hole alkali injection and single-hole alkali injection with a hole spacing of 6 m on the tunnel face. Under the same treatment effect, the construction time is significantly reduced compared with the single-hole. The simulation results can guide the prevention and control of H_2S emission disasters in the tunnel.

Keywords: H_2S, neutralization reaction, tunnel face, advanced alkali injection, lye injection simulation

1 INTRODUCTION

H_2S, a colorless, slightly sweet, stinky egg smell of acidic highly toxic gas [1], is one of the toxic and harmful gases in the tunnel. In recent years, the number of tunnel constructions in China has been increasing, and various complex geological conditions will be encountered in tunnel excavation [2]. H_2S gas overflow easily occurs during tunnel excavation and operation, causing casualties and economic losses [3]. H_2S governance has become a crucial issue in tunnel excavation. Huayingshan highway tunnel, Tianping tunnel of Chongqing-Guizhou railway, Huhanrong tunnel, and

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Caishen temple tunnel have encountered toxic and harmful gases such as H_2S and gas [4].

Domestic and foreign scholars have carried out a lot of research on dealing with the H_2S problem. Western scholars mainly use catalytic desulfurization to control H_2S in coal [5]. Chinese scholars control mine H_2S through air volume control and acid-base neutralization reaction [6]. Tang et al. [7] believed that the protection of H_2S in the tunnel has the problem of lack of protection or too much protection, and proposed a hierarchical protection system, which has been well used in the Micangshan tunnel. Lei et al. [8] established a numerical model based on the Huayingshan tunnel. Through the analysis of the ventilation flow field, the flow velocity threshold in the air duct that the low wind speed zone completely disappeared, and the H_2S concentration was significantly reduced. Chen [9] put forward the prevention and control measures for the non-coal gas tunnel from the aspects of gas and H_2S prevention and control in Hongdoushan tunnel. The problem of H_2S overrun can be solved from the source by the method of advanced alkali injection on the tunnel face.

In this paper, COMSOL Multiphysics software is used to numerically simulate the treatment of H_2S by injecting an alkali solution into the tunnel face. The migration and diffusion of alkali solution in the rock mass and the reaction law of $NaHCO_3$ solution and H_2S were analyzed. It has reference significance for the development of tunnel H_2S emission control technology.

2 NUMERICAL MODEL

The lye permeability in rock mass includes pressure seepage, capillary action, and diffusion. According to the fluid network theory, the lye flows first in the primary fractures of the rock mass. After that, the lye continues to spread around under the combined action of alkali injection pressure and capillary force. The neutralization reaction between the $NaHCO_3$ solution injected into the rock mass and the H_2S in the rock mass occurs. The chemical reaction equation is:

$$NaHCO_3 + H_2S \rightarrow NaHS + H_2O + CO_2 \tag{1}$$

The treatment of H_2S by alkali injection on the tunnel face is divided into two processes: alkali seepage and chemical reaction, and the following assumptions are made. (1) The rock mass contains many cracks and micro-pores; (2) The seepage and diffusion of each reaction substance conform to Fick's law; (3) The diffusion process of lye conforms to Darcy's law; (4) The physical and chemical properties of rock mass are isotropic; (5) The original H_2S content and temperature distribution in the rock mass are uniform.

2.1 Seepage Field Equation

According to References [10-11], the law of fluid flow in rock fracture is studied. The free seepage of fluid in fractures can be described by the N-S equation, and the seepage in micropores can be characterized by the Brinkman equation. The lye does not react with the rock mass structure, and the flow of the lye in the micro-pores of the rock mass satisfies the equation as follows:

$$\rho\frac{\partial u}{\partial t}+\nabla\cdot\left[-\mu\left(\nabla u+\left(\nabla u\right)^{T}\right)+pI\right]=-\rho\left(u\cdot\nabla\right)u \tag{2}$$

where μ is the viscosity of the fluid; u is the seepage velocity matrix of lye, and the seepage velocity is u; ρ is the density of rock mass; p is pressure; I is the unit diagonal matrix; and t is the reaction time.

The seepage and diffusion of lye in the micro-pores of rock mass satisfies the Brinkman equation as follows [11]:

$$\frac{\rho}{\varepsilon_p}\frac{\partial u}{\partial t}+\nabla\cdot\left[-\frac{\mu}{\varepsilon_p}\left(\nabla u+\left(\nabla u\right)^{T}\right)+pI\right]=-\frac{\mu}{k}u \tag{3}$$

$$u=-\frac{k}{\mu}\nabla p \tag{4}$$

where ε_p is the porosity of rock mass; k is the permeability matrix of rock mass, and the permeability is k.

2.2 Chemical Field Equation

The injected alkali solution is a low-concentration solution, and its diffusion conforms to Fick's law. The change of material concentration in the reaction satisfies the convection-diffusion process [12-13]:

$$\frac{\partial c_B}{\partial t}+\nabla\cdot\left(-D_B\nabla c_B+c_B u\right)=R_B \tag{5}$$

where c_B is the concentration of substance B; D_B is the diffusion coefficient of substance B; R_B is the chemical reaction rate of substance B; and u is the flow rate of lye.

The treatment of H_2S by injecting alkali into the tunnel excavation faces is essentially a neutralization reaction between OH^-ions hydrolyzed by alkali solution and H_2S. The reaction rate satisfies the Arrhenius equation is provided as follows:

$$R_{NaHCO_3}=R_{H_2S}=-Kc_{NaHCO_3}c_{H_2S} \tag{6}$$

$$R_{NaHS}=R_{H_2O}=R_{CO_2}=Kc_{NaHCO_3}c_{H_2S} \tag{7}$$

$$K = AT^n \exp\left(-\frac{E}{R_g T}\right) \tag{8}$$

where K is the chemical reaction rate constant, given by the Arrhenius equation [12]; A is the frequency factor; n is the index of temperature; E is the activation energy; R_g is the gas state constant; and T is temperature.

2.3 Definite Condition

Boundary Condition. The boundary conditions of alkali injection in the borehole include the flow rate u of alkali injection in the borehole, the pressure p_0 of alkali injection, and the concentration c_B of alkali injection.

Export quality transfer meets:

$$n\cdot\left(-D_B\nabla c_B + c_B u\right) = n\cdot c_B u \tag{9}$$

There is no convection-diffusion of reaction material in the rock structural plane:

$$n\cdot\left(-D_B\nabla c_B + c_B u\right) = 0 \tag{10}$$

Initial Condition. The initial concentration of H_2S in the rock mass is 32.8524 mol/m^3; the mass fraction of lye is 0.5 %; other parameters such as alkali injection pressure, rock mass density, and permeability are shown in Table 1.

Table 1. Model calculation parameters.

Parameter	numerical value	parameter	numerical value
μ/(Pa·s)	1.005×10^{-3}	$c(NaHCO_3)$/(mol·m^{-3})	59.5
ε_p/%	3.03	D_B/(m^2·s^{-1})	1.0×10^{-13}
u/(m·s)	3.977×10^{-3}	A/(m^3·mol^{-1}·s^{-1})	1.0×10^{-6}
ρ/(kg·m^{-3})	1.0×10^{3}	E/(J·mol^{-1})	7.2×10^{4}
p/MPa	2.0	R_g/(J·mol^{-1}·K^{-1})	8.314
k/mD	1.433×10^{-3}	p_0/MPa	0.26
$c(H_2S)$/(mol·m^{-3})	32.8524	T/K	298.15

2.4 Numerical Simulation

Geometric Model and Calculation Parameters. Taking Huayingshan Highway Tunnel as the research object, a model with a geometric size of 50m×40m×20m is established (Figure 1). The length of the model is 50 m, the inclination is 40 m, and the height is 20 m. The alkali injection borehole is drilled along the vertical rock wall, with an aperture of 100 mm and a depth of 30 m.

Through the physical parameter experiment of tunnel rock and the pre-injection alkali test on-site, the calculation parameters in the simulation are determined as shown in Table 1. The chemical properties of the injected alkalis are described in reference [12].

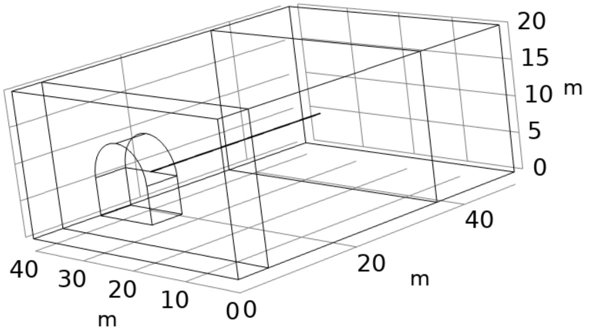
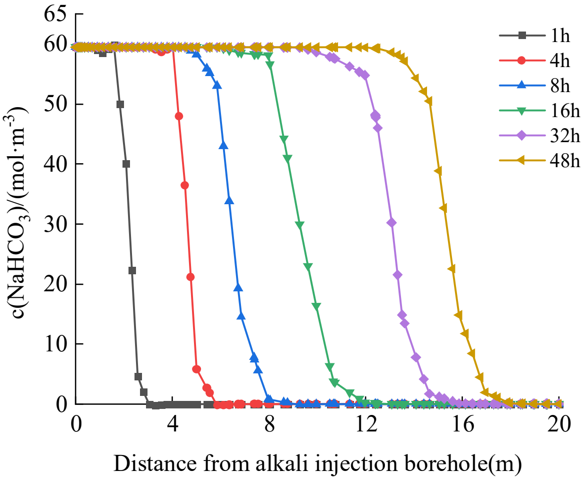


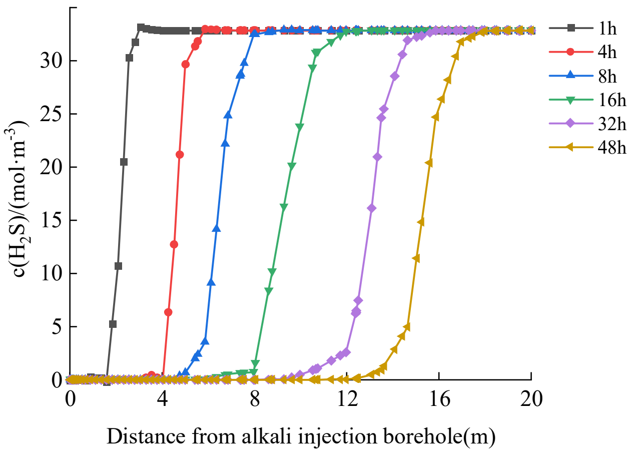
Fig. 1. Geometric model.

2.5 Numerical Simulation Results

Numerical Simulation of Single-Hole Alkali Injection. To analyze the seepage of lye in the rock mass during the alkali injection process and the change of H_2S content in the rock mass after alkali injection, the single-hole alkali injection simulation was first carried out. The variation curves of lye and H_2S content in rock mass after alkali injection for 1, 4, 8, 16, 32, and 48 h are shown in Figure 2. Due to the limited space, only the changes of lye and H_2S content in rock mass after 1h and 48h of alkali injection are given as shown in Figure 3. Figure 2 demonstrates that the influence range of lye gradually expands with the increase of alkali injection time, and the lye continuously penetrates the fracture of rock mass and reacts with the H_2S existing in the rock mass. The concentration of hydrogen sulfide in the rock mass area after alkali infiltration is significantly reduced. The closer to the alkali injection hole, the faster the alkali seepage, and the faster the H_2S concentration decreases.

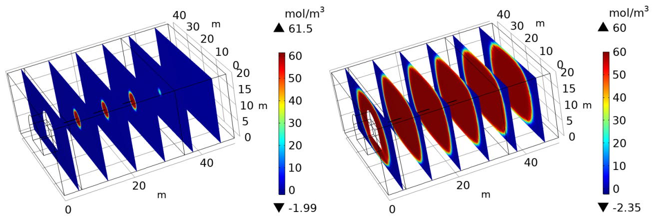


(a) Alkali liquor of rock mass

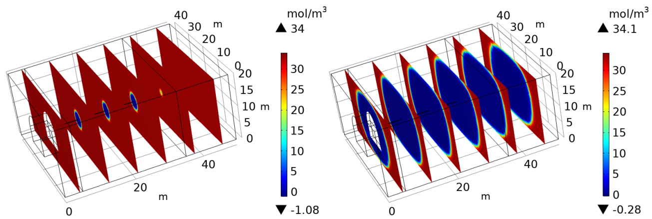


(b) Rock mass H_2S

Fig. 2. The variation curve of alkali solution and H_2S concentration with alkali injection time in rock mass.



(a) 1h, rock lye (b) 48h, rock lye

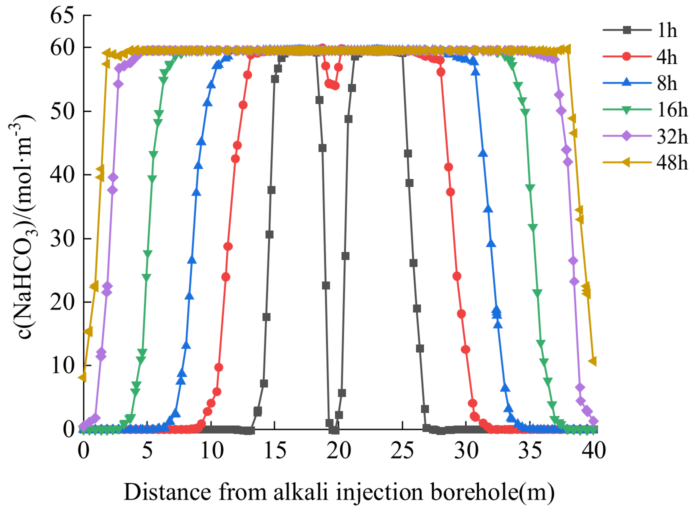


(c) 1h, rock H_2S (d) 48h, rock H_2S

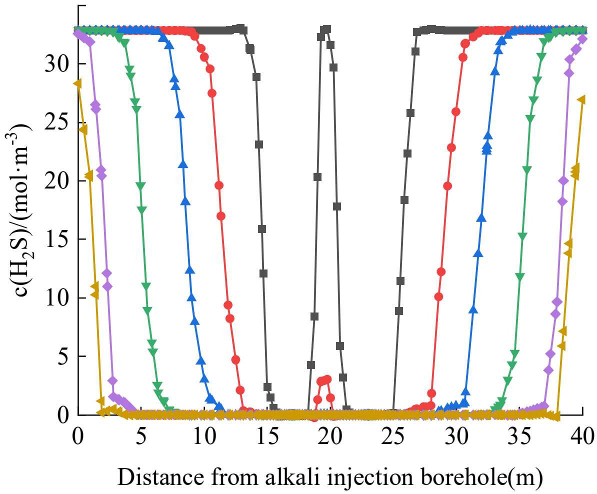
Fig. 3. The concentration of alkali solution and H_2S in rock mass changes with alkali injection time.

After 1h of alkali injection, the alkali solution flows to the position of 1~2 m away from the hole. About 1m away from the hole, the alkali concentration reached 58 mol/m^3. After 4 hours of alkali injection, the lye affects the drilling range of 4 m. 4 m away from the hole, the alkali concentration is about 48 mol/m^3. The concentration of hydrogen sulfide decreased to 6 mol/m^3, decreased by 81.7 %. After 8h of alkali injection, the concentration of H_2S decreased at different degrees in the range of 6 m from the borehole. The concentration of alkali solution reached 50 mol/m^3 and the concentration of H_2S decreased to about 6 mol/m^3 at 6 m from the hole. After 16 h of alkali injection, H_2S is nearly completely neutralized within 8 m from the hole. The concentration of lye is about 35 mol/m^3, and the concentration of H_2S is 14 mol/m^3, which is reduced by 57.4 %. After 32 h of alkali injection, H_2S is nearly completely neutralized within 10 m. The concentration of the alkali solution was 30 mol/m^3 and the concentration of hydrogen sulfide was 16 mol/m^3, which was reduced to 48.7 % of the original concentration. After 48 h of alkali injection, the influence range of the alkali solution was about 17 m, and H_2S was completely neutralized in the range of 12 m from the hole.

Numerical Simulation of Double-Hole Alkali Injection. In addition to single-hole alkali injection, this paper also carried out a numerical simulation analysis of double-hole alkali injection with a hole spacing of 6 m. According to the occurrence of H_2S in the rock mass, the effect of alkali treatment of H_2S in parallel double holes with a hole spacing of 6 m was simulated and analyzed. Figure 4 shows the change curve of alkali and H_2S content in rock mass after alkali injection for 1, 4, 8, 16, 32, and 48 h respectively when alkali injection is carried out at 6 m hole spacing. The variation of lye and H_2S concentration with alkali injection time after continuous alkali injection for 1 h and 48 h are shown in Figure 5.

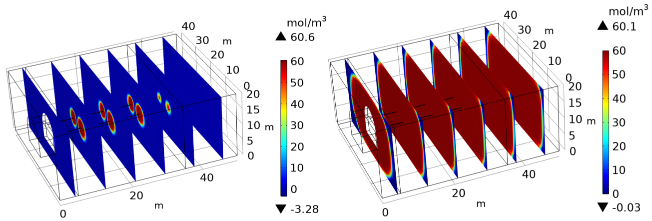


(a) Alkali liquor of rock mass

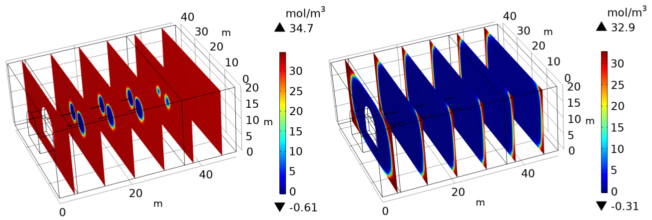


(b) Rock mass H_2S

Fig. 4. The variation curve of alkali solution and H_2S concentration with alkali injection time in rock mass



(a) 1h, rock lye (b) 48h, rock lye



(c) 1h, rock H_2S (d) 48h, rock H_2S

Fig. 5. The concentration of alkali solution and H_2S in rock mass changes with alkali injection time.

It can be seen from Figure 4 that after 1 h of alkali injection, the H_2S concentration of rock mass in the range of 3 m from the borehole decreased to varying degrees. About 2 m away from the borehole, the concentration of H_2S dropped to less than 2.5 mol/m^3. After 4 h of alkali injection, the concentration of H_2S in the range of 8 m from the borehole decreased to varying degrees. H_2S was completely neutralized in the range of 4 m from the borehole. After 8 h of alkali injection, H_2S was completely neutralized in the range of 6 m around the borehole. After 16 h of alkali injection, H_2S was completely neutralized in the range of 9 m around the borehole. After 32 h of alkali injection, H_2S was completely neutralized in the 12 m range around the borehole. After 48 h of alkali injection, H_2S was completely neutralized in the range of 13 m around the borehole. After 32 h of alkali injection, the influence range of alkali injection did not increase significantly with the increase of alkali injection time. It is suggested that the double-hole alkali injection time should be about 32 h. Too long a time will affect the progress of tunnel excavation.

According to the simulation results, the construction time is significantly reduced compared with the single hole when the alkali injection hole spacing is 6 m. On the other hand, it can also try to increase the hole spacing within a reasonable range. Improve the utilization rate of drilling lye, and then improve the progress of H_2S treatment. Due to the limited space, this paper only simulates and analyzes the hole spacing of 6 m. The numerical simulation analysis of alkali injection with different hole spacing will continue in the future. To determine the reasonable hole spacing when multiple boreholes are injected with alkali at the same time. It provides a reference for tunnel construction.

3 CONCLUSIONS

(1) The mathematical model of H_2S treatment by alkali injection in rock mass is established, including the seepage field and chemical field. The N-S equation is used to describe the free flow of lye in rock fractures, and the Brinkman equation is used to describe the seepage of lye in rock micropores. The concentration change of the material reaction is described by the convection-diffusion equation, and the reaction rate satisfies the Arrhenius equation.

(2) The simulation results show that when the alkali is injected into the tunnel face, the influence range of alkali injection increases with the increase of alkali injection time. The closer to the alkali injection borehole, the faster the alkali seepage migration, and the farther the distance, the slower.

(3) In the rock mass area infiltrated by lye, the concentration of hydrogen sulfide is significantly reduced. After 16 h of alkali injection, H_2S is nearly completely neutralized within 8 m from the alkali injection hole. The content of H_2S decreased by 57.4 %~95.4 % compared with that without lye injection at 8-9 m from the borehole. After 32 h of alkali injection, H_2S was neutralized within 10 m of the alkali injection borehole. The H_2S content is reduced to less than 48.7 % in the range of 13 m from the borehole.

(4) When double boreholes are injected with alkali, the construction time is significantly reduced compared with a single borehole under the same treatment effect. After 32 h of alkali injection, the influence range of alkali injection did not increase significantly with the increase of alkali injection time. It is recommended that the double-hole alkali injection time should be controlled at about 32 h. Due to the lim-

ited space, this paper only simulates and analyzes the effect of alkali injection on the hole spacing of 6 m. In the future, the numerical simulation analysis of alkali injection with different hole spacing will be continued to improve the efficiency of H_2S treatment.

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