Effect of Water on the Chain Reaction Characteristics of Gas Explosion
Xiangchun Li, Huan Zhang,* Chunli Yang, Jianfei Zhao, Sheng Bai, and Yuzhen Long

ABSTRACT: In order to explore the influence of water on the chain reaction characteristics of gas explosion, the 20 L explosion ball experiment and the homogeneous constant volume combustion reactor of CHEMKIN 17.0 simulations were carried out. The gas explosion response under four different water contents was tested and simulated. The effects of water on the pressure, free radicals, and reactants of gas explosion were compared and analyzed. The research results show that the inhibition of water on gas explosion was enhanced with the increase of water fraction in the initial mixture; the temperature, pressure, catastrophic gases such as CO, and concentration of activation centers in the reaction system can be reduced by water; the intensity of gas explosion can be reduced by inhibiting the formation of H, O, and OH free radicals, the main reactants of gas explosion and gas explosion energy.

1. INTRODUCTION

As the largest coal-producing country in the world, China’s coal output has been slowly declining in recent years due to various factors such as the speed of economic development and the adjustment of energy structure. Its annual coal output has dropped from 3.974 billion tons in 2013 to 3.546 billion tons in 2018. However, with the high production of coal, accidents occur frequently in the production process, threatening the safety of the mine and endangering the physical and mental health of workers. Coal mines, dangerous chemicals, fireworks, and noncoal mines are listed as four high-risk industries that threaten the safety of production in China. Preventing the occurrence of gas explosion accidents is still the focus of coal mines. It is of great significance to study the mechanism of water inhibiting gas explosion.

Many scholars and experts at home and abroad have done a lot of theoretical and experimental research on gas explosion. Thomas et al. used high-speed photography to observe the process of breaking shock droplets from explosion shock waves through an observation window parallel to the water mist zone in an opaque square flame tube with a length of 5.32 m and a cross-section of 175 mm × 275 mm. They found that the suppression effect of water mist on the explosion flame not only depends on the evaporation of the water mist but also the heat transfer and mass transfer caused by the initial water mist droplet breakage in the induced flow field before the flame array in the combustion zone. van Wingerden and Wilkins conducted an experimental study on the effect of water mist suppression of explosive flames in a rectangular steel tube. The experimental results show that under open explosion conditions, the flame acceleration is faster than in a closed environment, and the accelerated flame overpressure causes the water droplets to break, which causes the explosion flame to fall overpressure. Lu and He analyzed the chemical reaction kinetics of water involved in gas explosion and calculated the equilibrium by explosion reaction and stated that water acts as a third carrier or an inert droplet to destroy the chain carrier in the gas explosion chain reaction process, thereby reducing the gas explosion reaction capability. The gas content of the gas mixture increases, the gas explosion capacity decreases, the strength decreases, and the explosion limit concentration range decreases. Deng et al. conducted a detailed study on the microscopic dynamics and thermodynamics of gas explosions; Wang and Chen used the theory of chemical reaction kinetics combined with detailed gas explosion reaction mechanism and analyzed the influence of water and CO₂ in the enclosed space on the kinetic characteristics of the gas explosion reaction. Su et al. used density functional theory (CAMB3LYP/6-31g) and a detailed mechanism (GRI-Mech 3.0) to deeply study the chemical kinetic behavior of the initial stage of the explosion of

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the CH4/H2/air mixture and obtained the reaction mechanism of the key reaction. It was found that the addition of H2 increased the laminar combustion speed and shortened the ignition delay time of the H2/CH4/air mixture. The research results can provide theoretical and technical guidance for the research on water suppression of gas explosion. Li and Luo et al.15 took the key product of methane explosion chain reaction (CH2O) as the research object and proposed a method to analyze the coupling mechanism of explosion pressure and intermediate products. This method provides a theoretical basis for the construction of an explosion control system with chemical effects. Yang16 analyzed the evaporation endothermic of water spray droplets during the fire extinguishing process and found that the evaporation time of the water droplets was proportional to its diameter. The larger the diameter, the longer the evaporation time and the longer the heat absorption time. Liu et al.17 used a self-developed flame propagation tube experimental system and a water spray system to conduct experimental research on the gas flame propagation process under different water mist conditions. It was found that the water mist acts on the reaction zone of the flame front, so that the gas combustion reaction speed is weakened, the preheating zone of the flame front is prolonged, the heat transfer and mass transfer of the flame front are slowed down, and hence the propagation flame is suppressed. The research of Xu et al.18 shows that water can react with free radicals and inhibit the chain reaction in gas explosion suppression besides cooling down. Wang et al.14 used a cylindrical device to experimentally study the influence of combustible gas and relative humidity (RH) on the flammability limit behavior of methane under various RHs; they used the theoretical model based on the adiabatic flame temperature method to estimate the flammable limit of methane and steam mixture. It was found that the flammability limit of methane increased with the increase of RH, and water vapor and gas changed the initial chain reaction of methane/air. Luo15 combined the Gaussian software to analyze the microscopic thermodynamics and kinetics of gas explosion chain reaction and analyzed the explosion suppression mechanism of mine gas explosion from the perspectives of cooling, shielding barrier, and homogeneous inhibition. After that, he and Hao et al.16 studied the propagation characteristics of methane/ethane/air premixed explosion by using a horizontal closed pipe and a high-speed camera; they studied the evolution characteristics of the flow field in the pipeline during the explosion propagation by numerical simulation and obtained the variation law of the premixed flame propagation speed by using the program written by the Canny operator. The results show that ethane increases the reaction rate and explosion intensity of premixed gas. Bi17 and Zhang18 experimentally studied the relationship between the spray volume and gas explosion pressure and ascending rate and proved the inhibition of water on gas explosion. Yu19 and Xu et al.20 studied the inhibiting effect of charged water mist on gas explosion. Xue and Huang21 studied the effect of fine water mist particle size on gas explosion and found that the fine water mist particle size of about 190 μm has better antiexplosion effect. Li and Zeng22 used CHEMKIN to carry out numerical simulation of gas explosion and studied the inhibition of water on gas explosion. Tang23 used FLUENT and CHEMKIN to simulate the suppression of water mist on the gas explosion temperature and pressure.

In recent years, it has been found that the flameproof water shed which has been used to prevent the accidental spread of coal dust explosion has a certain hindrance effect on gas explosion. Hence, the experimental study on the effect of water on the reaction characteristics of gas explosion has been started, and the numerical simulation has been applied to the study and analysis of the law of gas explosion. Compared with the one-step macroscopic reaction process used in most previous studies, analyzing the mechanism of action of water inhibiting gas explosion from a microscopic point of view can help us understand more clearly the mode of action of water, and numerical simulation can help us systematically analyze the suppression effect of water on gas explosion from a microscopic point of view. At present, the main software used for gas explosion simulation research are AutoReaGas, FLUENT, PHOENICS, CHEMKIN, and so forth. CHEMKIN can study the mechanism of gas explosion more deeply and in detail. Therefore, this article will use a multistep detailed reaction mechanism to study the chain reaction characteristics of gas explosion combined with the macro characteristics and analyze the way of the effect of water on the whole process of gas explosion from the microlevel, so as to provide theoretical support and breakthrough point for finding methods to improve the effect of water in suppressing the gas explosion. At the same time, it provides new ideas for finding more efficient explosion suppression materials from the perspectives of inhibiting chain reactions, reducing free radicals, and reducing the generation of explosive products in order to make further explorations for gas explosion prevention and suppression.

2. EXPERIMENT ON GAS EXPLOSION SUPPRESSION BY WATER

This experiment uses a 20 L spherical explosion test system, as shown in Figure 1. The experimental system mainly includes a

![Figure 1. Schematic diagram of a 20 L spherical explosive device.](https://doi.org/10.1021/acsomega.1c00153)
supply source, water storage tank, pressure gauge, solenoid valve, one-way valve, pipeline, and atomizing nozzle. This experiment mainly studies the inhibition effect of water contents of 0, 1, 2, 3, and 4 mL on gas explosion. In the experiment, pure water was injected into the powder storage bin by manual water injection, and methane air-premixed gas was injected into the spherical explosive device by direct gas distribution. The volume fraction of methane was 9.5%. After the mixed gas in the device was left standing for half a minute, the solenoid valve switch of the gas storage chamber was opened by the control system, and the water mist generated by the water mist generation device was transported to the explosion device by using compressed air, and the ignition was triggered after a delay of 100 ms. At the same time, the data acquisition system was triggered to collect experimental data.

3. GAS EXPLOSION MODEL

3.1. Physical Model and Mechanism. When selecting the simulation kinetic model corresponding to the experimental device, it is necessary to consider that the simulated conditions are always better than the actual experimental conditions. Therefore, when choosing the kinetic model of the simulation software, only the reactor that matches the experimental equipment as much as possible can be selected. Through the summary and comparison of previous studies, combined with the actual selection of the explosive ball experimental device and the parameter data required for this study, a CHEMKIN 17.0 built-in closed homogeneous batch reactor was chosen as the model for simulation. The model was a 0D constant volume, sealed adiabatic model with a uniform distribution of material components in the reactor and unchanged total molecular weight. The simulated mechanism document is the GRI-Mech 3.0 methane explosion mechanism document which is internationally recognized and considered to be the most reliable by Lawrence Livermore, including gas phase dynamics file grimech3.0_chem.inp, thermodynamic data file grimech3.0_thermo.dat, and gas transport data file grimech3.0_transport.dat. Initially, GRI-Mech had only 12 components and 15 elementary reactions. With the deepening of research and the continuous optimization of software, it has developed to the present 53 components and 325 elementary reactions.

3.2. Computational Model. According to the selected physical model, the following basic assumptions are made to establish the gas explosion calculation model: (1) the gas is inviscid and satisfies the equation of state of an ideal gas; (2) the wall is rigid and does not consider the fluid—solid coupling with gas flow; (3) there is no heat exchange between the system and the system.

3.2.1. Control Equation. Reactors, intermediates, and products at any position in a constant volume combustion reactor all react at the same rate, that is, there is no temperature and concentration gradient distribution, so the overall change of the system can be described by a set of component concentration parameters and a temperature parameter. The relationship between the component concentration and temperature can be obtained by the following equation.

3.2.1.1. Component Equation.

\[
\frac{dY_i}{dt} = \nu \dot{\omega}_i W_i \quad (i = 1, ..., g)
\]  

\[
\dot{\omega}_i = \sum_{k=1}^{n} v_{ik} s_k \prod_{i=1}^{g} X_i^{y_{ik}} \quad (i = 1, ..., g)
\]  

\[
s_k = A_k T^{b_k} \exp \left( -\frac{E_{ak}}{RT} \right) \quad (k = 1, ..., n)
\]

where \(Y_i\) is the mass fraction of component \(i\), \(W_i\) is the molecular weight of species \(i\), \(\nu\) is the reaction rate of component \(i\), \(\dot{\omega}_i\) is the reaction rate of \(\dot{\omega}_i\); \(v\) is the specific heat capacity of the whole mixed gas, \(J/(kg\cdot K)\); \(g\) is the total number of gas components; \(n\) is the total number of reaction steps; \(X_i\) is the molar concentration of component \(i\), \(mol/L\); \(s_k\) is the positive rate constant in the \(i\)-th reaction; \(A_k\) and \(b_k\) are the preexponential factors and temperature indices of the \(i\)-th reaction; \(E_{ak}\) is the activation energy of the \(i\)-th reaction, \(J/kmol\); \(T\) is the temperature of mixed gases, \(K\); \(R\) is the mixed gas constant, \(J/(kg\cdot K)\).

3.2.1.2. Energy Equation.
Fraction ratio of air $79/21$. The calculation of the volume concentration of methane is 9.5%, and the molar fraction of oxygen, and nitrogen in the scheme remains unchanged, the order to increase the comparability, the ratio of methane, energy equation, and adiabatic condition, without heat loss. In source to ignite. The problem type is constant volume, solving conditions was simulated with a 1200 K high temperature heat source.

Figure 3. Effect of water on the final concentration of residual reactants and products. (a) Experimental results. (b) Simulation results.

\[ c_v \frac{dT}{dt} + p \frac{dv}{dt} + \nu \sum_{i=1}^{k} \epsilon_i \dot{W}_i = 0 \]  

where $p$ is the mixed gas pressure, $P_a$; $c_v$ is the specific heat capacity of mixed gas at a constant volume, J/(kg·K); $t$ is the time, $s$; $\epsilon_i$ is the internal energy of component $i$.

3.2.2. Sensitivity Analysis Equation. It is very important to understand the mechanism of gas explosion that the key reaction promotes or inhibits in the total package reaction in the process of gas explosion. For the explosive reaction system, sensitivity analysis can reflect the magnitude of each characteristic variable changing with the rate of elementary reaction step. Assuming a variable $Z_i$ the governing equation is as follows 

\[ \frac{dZ_i}{dt} = F(Z, t, a) \]  

where $Z = (Y_1, Y_2, ..., Y_n)^T$ is the mass fraction of each component; $a = A_1, A_2, ..., A_n$ is the preexponential factor.

The coefficient of sensitivity can be obtained by the following formula

\[ q_{i,k} = \frac{\partial Z_i}{\partial a_k} \]  

where $q_{i,k}$ is the coefficient of sensitivity; $Z_i$ is the $l$-th variable; $a_k$ is the preexponential factor of the $k$-th reaction.

3.3. Initial Calculation Conditions. The calculation model is a homogeneous constant volume combustion reactor. The initial gas air mixture was filled with 0, 1, 2, 3, and 4 mL of moisture, and the gas explosion under different moisture conditions was simulated with a 1200 K high temperature heat source to ignite. The problem type is constant volume, solving energy equation, and adiabatic condition, without heat loss. In order to increase the comparability, the ratio of methane, oxygen, and nitrogen in the scheme remains unchanged, the concentration of methane is 9.5%, and the molar fraction of nitrogen and oxygen is calculated according to the volume fraction ratio of air $79/21$.

4. RESULTS

4.1. Effect of Water on Pressure. The effect of water on the final pressure after gas explosion is shown in Figure 2.

From the experimental results and simulation results in Figure 2, it can be seen that when the gas concentration is constant, within a certain range of water content, the maximum gas explosion pressure decreases with the increase of water content, that is, the gas explosion pressure is negatively correlated with the water content. The higher the water content, the better the inhibition effect of water on gas explosion. The addition of water weakens the intensity of gas explosion and reduces the harm of explosion. From the macroscopic parameters, water has an obvious inhibition effect on gas explosion.

Compared with Figure 2a, b, it can be seen that under the initial simulation conditions, the pressure at the end of gas explosion decreases with the increase of water and shows an approximate linear downward trend. The experimental results show that the inhibition effect of gas explosion pressure changes slowly when the water content is 2–4 mL. This is because under the experimental conditions, when the water content is more than 2 mL, due to the limitation of the air pressure in the powder storage tank during the experiment, the water mist cannot all become fine water mist particles, so the maximum explosion pressure of water is not significantly reduced. However, in the simulation, the setting of initial conditions is ideal and will not be affected by the concentration of water added before.

4.2. Effect of Water on Gas Explosion Reactants and Products. The effect of water on the final residual reactant and final product concentration is shown in Figure 3.

From the experimental results and simulation results in Figure 3, it can be seen that within a certain range of water content, the final residual concentrations of CO$_2$ and O$_2$ decrease with the increase of water content, while the final residual concentrations of CH$_4$ and CO increase with the increase of water content. When no water is injected into the constant volume container, the gas explosion combustion reaction in the container is fuel–lean combustion, so the gas in the mixed gas can fully carry out the explosion combustion with oxygen; the gas residue is very small, and there is almost
no gas residue under the simulated ideal conditions. After injecting water into the container, when the gas concentration remains unchanged with the increase of water content, the O2 content in the mixed gas decreases relatively, and water participates in the gas explosion reaction, which promotes the reverse reaction. Therefore, with the increase of water content, the residual gas content in the tail gas increases. Compared with Figure 3a,b, it can be seen that under the initial simulation conditions, the overall content of residues and products after gas explosion reaction is much lower than that under the experimental conditions, which is also because the initial conditions in the simulation are relatively ideal.

### 4.3. Effect of Water on the Free Radical

In the gas explosion chain reaction, O, H, and OH are the main free radicals which could dominate the rate of reaction. The final concentration changes of O, H, and OH are shown in Figure 4.

It can be seen that within a certain range of water content, the final free radical concentration after gas explosion decreases with the increase of the initial water content, and the more the water content, the more obvious the effect of suppressing the gas explosion. Active radicals such as hydrogen radicals, oxygen radicals, and hydroxyl radicals are the chain reaction transmitters (key chain carriers). These radicals will then aggregate into higher active centers, thereby increasing the intensity of the entire reaction. Therefore, the effect of water on the concentration of such radicals can inhibit the explosion reaction and reduce the intensity of the explosion reaction.

### 5. DISCUSSION

#### 5.1. Effect of Water on the Main Reactants of Gas Explosion

The effect of water on the main reactants of methane explosion is the macroscopic manifestation of the effect of water on the microreaction process of methane explosion. In this section, the change of the sensitivity coefficient of the key element reaction under different water content conditions is used to discuss and analyze the results combined with the element reaction path. Figure 5 shows the sensitivity coefficients of the key elementary reaction.

The main reaction steps to inhibit methane consumption are R53: H + CH4 → CH3 + H2; R98: OH + CH4 → CH3 + H2O; R57: H + CH3O(+M) → CH2O(+M); R161: CH3 + CH3O → HCO + CH4; R158: 2CH3(+M) → C2H6(+M).

The key reaction steps to promote methane consumption are R38: H + O2 → O + OH; R155: CH3 + O2 → O + CH2O; R119: HO2 + CH3 → OH + CH2O; R156: CH3 + O2 → OH + CH2O; R170: CH3O + O2 → HO2 + CH2O; R101: OH + CH3O → HCO + H2O.

In the key elementary reactions affecting methane explosion, R38 and R53 are important chain initiation reactions, R32, R119, R155, R156, R161, and R170 provide oxidation and reduction pathways of CH4, and R158 is the chain termination reaction. Among them, R32, R35, R38, R101, R119, R155, R156, R161, and R170 play an important role in CH4 consumption by promoting the manufacture of free radicals, while R53, R57, R98, R118, and R158 can inhibit the consumption of CH4 by consuming free radicals.

It can be seen from Figure 5 that water can change the sensitivity of the key element reaction. With the increase of the water content, the peak value of the sensitivity coefficient of the key element reaction is smaller and smaller, and the peak arrival time is also delayed. In the key elementary reaction that inhibits CH4 consumption, the sensitivity of R158 is far greater than that of other compounds, and the inhibitory effect is more obvious. In the key elementary reaction that promotes CH4 consumption, the sensitivity of R38 decreases relatively significantly. The sensitivity of other key elementary reactions has been reduced but relatively insignificant. The sensitivity of the methane radical reaction is mainly affected by the properties of reactants, concentration, temperature, pressure, catalyst, and other external factors. According to the analysis of the effect of water on the main free radicals H, O, and OH in the chain reaction theory, the addition of water can inhibit the number of free radicals. In the process of methane explosion, H, O, and OH radicals are the key components to ensure the smooth progress of the reaction; especially in the initial stage of the reaction, they play an important role in the basic reaction. In addition, it can be seen from the simulation results that the addition of water can reduce the sensitivity of explosion reaction and the rate of elementary reaction. Therefore, the addition of water can reduce the sensitivity of the reaction step.
In the methane explosion reaction, the main formation reactions of CH₃ radicals are R53 and R98, and with the increase of water content, the number of OH radicals decreased, but the proportion of OH radicals in methane explosion increased, resulting in a significant increase in the proportion of reaction R98 in the reaction of CH₃ formation.

Figure 5. (a) Effect of 0 mL of water on the key element reactions affecting CH₄ concentration. (b) Effect of 1 mL of water on the key element reactions affecting CH₄ concentration. (c) Effect of 2 mL of water on the key element reactions affecting CH₄ concentration. (d) Effect of 3 mL of water on the key element reactions affecting CH₄ concentration. (e) Effect of 4 mL of water on the key element reactions affecting CH₄ concentration. (f) Effect of 5 mL of water on the key element reactions affecting CH₄ concentration. (g) Effect of 6 mL of water on the key element reactions affecting CH₄ concentration.
The proportions of R119, R155, and R156, the main consumption reactions of CH₃ radicals, increased in the explosion process of aqueous methane, and more CH₃ radicals were converted into CH₂O radicals. The reaction R156 converts a larger proportion of CH₃ into CH₂O, which significantly increases the proportion of reaction R57. In addition, the increase in the proportion of OH radicals also increases the proportion of reaction R101, which promotes the increase in the proportion of CH₂O being consumed to produce HCO.

From the analysis of the above results, it can be seen that the addition of water will change the microscopic reaction process in the explosion process of methane. The main reaction process of methane explosion is CH₄ → CH₃ + H₂O → CH₂O + CO → CO₂; after the addition of water, the proportion of OH radical reaction increases in all free radicals, which strengthens the chain reaction process of OH radical transfer and thus increases and strengthens the CH₃ → CH₂O → CH₃O process. On the one hand, it increases the consumption of O₂ and makes the content of O₂ decrease gradually with the increase of water content; on the other hand, the increase of these reaction processes enhances the elementary reactions that inhibit the consumption of CH₄, such as R53, R57, and R98, and inhibits the elementary reactions that promote the consumption of CH₄, such as R38, so that the residual amount of methane after explosion increases with the increase of water content.

5.2. Effect of H₂O on the Free Radical Concentration in Gas Explosion. Chemical reactions can only occur when the activated molecules with activation energy contact and collide with each other.⁵⁵ According to the theory of free radical chain reaction,⁵⁴ there exists a chain carrier or a free radical with a catalytically active intermediate in the gas phase reaction system. This free radical has higher energy, is extremely mobile, and is very unstable. Once the reaction begins, the free radicals do not disappear, and the reaction continues until the reaction is complete or interrupted by other reaction steps.

Mine gas explosion reaction is a complex oxidation reaction, which belongs to the branched chain reaction. The relationship between the number of free radicals in the reaction and time is as follows:\(^{(7)}\)

\[
\frac{dW}{dt} = W_1 + W_2 - W_3 = W_1 + (f - g) \times n
\]

where \(W_1\) is the rate of generation of free radicals; \(W_2\) is the growth rate of free radicals; \(W_3\) is the rate of destruction of free radicals; \(f\) is the reaction rate constant of the radical generated by the branched chain; \(g\) is the rate constant of the chain termination reaction; \(n\) is the concentration of free radicals.

Because the initiation process is very difficult, the rate of generation of free radicals in the chain initiation process is generally small and negligible.

\[
\frac{dW}{dt} = W_1 + W_2 - W_3 = (f - g) \times n
\]

Finally, the reaction rate of gas explosion is \(W \sim d_W/d_t\).

Before the gas explosion reaction occurs, the concentration of free radicals rises sharply in a very short time, thereby forming a high concentration of activation centers. H₂O has a large specific heat capacity and absorbs more heat when participating in the reaction. With the addition of water, the time for radical quantity to rise sharply was delayed, and the more the water is added, the longer the delay. The bond energy of O–H bond in H₂O is 497.10 ± 0.29 kJ/mol, the bond energy of O–O bond in O₂ is 498.36 ± 0.17 kJ/mol, and the N–N bond energy in N₂ is 945.33 ± 0.59 kJ/mol. It can be seen that the O–H bond is more likely to break than the O–O bond and the N–N bond to form a radical, which means that H₂O is more likely to participate in the reaction than O₂ and N₂.

In the reaction, H₂O molecules can participate in the reaction process as reactants. For example, water molecules can interact with free radicals, H and O, such as R41: 2H + H₂O = H₂ + H₂O, H + H₂O → H₂ + OH, O + H₂O → 2OH, HO + H₂O → H₂O₂ + OH, which will reduce the proportion of active radicals such as H and O. Increasing the water content in the initial gas increases the probability of collision between water and active free radicals. All these cause the system’s free radicals (active centers) to drop, causing the chain reaction to terminate. Some water molecules act as a third body to enhance the three-body reaction in the gas combustion reaction mechanism under high temperature and pressure. These three-body collision reactions transfer the energy of a large number of free radicals or atoms to the third body-stabilizing molecule, thereby reducing the activity of the branching chain reaction.⁵⁶ Within a certain range, as the amount of H₂O added increases, the three-body collision reaction also enhances, making the reaction easy to proceed in the direction of generating a stable state. Therefore, the concentration of the final radical decreases with the increase of initial water content after the reaction.

5.3. Effect of H₂O on the Gas Explosion Energy and Activation Energy. The thermochemical equation of gas explosion reaction is as follows:

\[
\text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O}(l)
\]

\[\Delta H = -890.3 \text{ kJ/mol}\]  \((9)\)

Table 1 lists the elementary reaction steps and their activation energies involved in the 325 elementary reactions of the gas explosion reaction. These reactions consume a considerable amount of energy in the reaction system. As the proportion of water added increases, the promotion of these reactions also increases, increasing the energy consumption during the reaction. Therefore, the addition of water will reduce and consume the energy released by the gas explosion reaction, thereby suppressing the danger of gas explosion.

Activation energy is the amount that characterizes the ease of chemical reaction; \(\text{CH}_4 + \text{O}_2 \rightarrow \text{CH}_4 + \text{HO}_2\) is the rate-determining step of the chain initiation process with an

| number of reaction | equation | \(E\) (cal/mol) |
|-------------------|----------|-----------------|
| R35               | H + O₂ + H₂O → HO₂ + H₂O | 0.0            |
| R41               | 2H + H₂O → H₂ + H₂O         | 0.0            |
| R127              | CH + H₂O → H + CH₂O         | -755           |
| R148              | CH₂(S) + H₂O → CH₂ + H₂O   | -570           |
| R166              | HCO + H₂O → H + CO + H₂O   | 17,000         |
| R197              | NH + H₂O → HNO + H₂         | 13,850         |
| R219              | CN + H₂O → HCN + OH        | 7460           |
activation energy of 289.64 kJ/mol. It is difficult to carry out the chain initiation process of generating free radicals by stable molecular decomposition in the gas explosion reaction involving H2O. According to the Arrhenius formula

\[ K = K_0 \exp\left(-\frac{E_a}{RT}\right) \]  
(10)

\[ E_a = -RT\ln K - \ln K_0 \]  
(11)

where \( K \) is the rate constant; \( R \) is a molar gas constant with a value of 8.31441 ± 0.00026 J/(mol-K); \( T \) is the thermodynamic temperature; \( E_a \) is the apparent activation energy; \( K_0 \) is the preexponential factor (also called the frequency factor).

The activation energy of the reaction can be calculated by measuring the rate constants at two different temperatures during the reaction. During the gas explosion, the activation energy required for H2O participation is lower than the activation energy required for some other intermediates to participate in the reaction. Therefore, the addition of water will cause the relevant reaction to proceed, blocking some other intermediates to participate in the reaction, thereby changing the reaction direction of the gas explosion and reducing the gas explosion hazard. For example, the activation energy of R126, \( CH + H_2 \rightarrow H + CH_2 \), is 1670, and the activation energy of R127, \( CH + H_2O \rightarrow H + CH_2O \), is ~755. The addition of H2O promotes the equilibrium shift of the R127 reaction to the right while inhibiting the R126 reaction.

6. CONCLUSIONS

(1) After being added to gas explosion, water can reduce the final pressure of the gas explosion from the macroscopic view. The addition of water, on the one hand, reduces the content of O2 in the mixed gas; on the other hand, it promotes the reverse reaction, thus increasing the content of CH4 and reducing the concentration of CO2 and other important products.

(2) Water reduces the participation of the main reactants by reducing the sensitivity of key reaction steps of main substances and reduces the concentration of main free radicals by inhibiting the formation and collision of main free radicals, which have a certain suppressive effect on the chain reaction of gas explosion on the microlevel.

(3) Since the activation energy required for H2O participation is relatively low, the addition of water blocks some other intermediates from participating in the reaction, thereby changing the reaction direction of the gas explosion and reducing the gas explosion hazard. As the proportion of water added increases, the elementary reaction of water participates in consuming a considerable amount of energy in the reaction system, thereby suppressing the hazard of gas explosion.

AUTHOR INFORMATION

Corresponding Author

Huan Zhang – College of Emergency Management and Safety Engineering, China University of Mining and Technology, Beijing 100083, China; orcid.org/0000-0002-0614-7412; Phone: 15300220145; Email: zhanghuan19kd@163.com

Authors

Xiangchun Li – College of Emergency Management and Safety Engineering, China University of Mining and Technology, Beijing 100083, China; State Key Laboratory of Coal Resources and Safe Mining, Beijing 100083, China; State Key Laboratory of Coal Resources and Safe Mining, Beijing 100083, China; State Key Laboratory of Coal Resources and Safe Mining, Beijing 100083, China; State Key Laboratory Cultivation Base for Gas Geology and Gas Control, Jiaozuo 454000, China

Chunli Yang – Occupational Hazards Control Technology Center, Beijing Municipal Institute of Labor Protection, Beijing 100054, China

Jianfei Zhao – College of Emergency Management and Safety Engineering, China University of Mining and Technology, Beijing 100083, China

Sheng Bai – College of Emergency Management and Safety Engineering, China University of Mining and Technology, Beijing 100083, China

Yuzhen Long – College of Emergency Management and Safety Engineering, China University of Mining and Technology, Beijing 100083, China

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.1c00153

Notes

The authors declare no competing financial interest.

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