

Numerical simulation of the influence of water vapor on gas explosions in a high-pressure environment

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Research

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Numerical simulation of the influence of water vapor on gas explosions in a high-pressure environment

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Abstract Gas explosion seriously threaten the employees security and restrict the safe production of coal mines. Therefore, it is particularly essential to investigate the prevention and control of gas explosions. In this study, a two-dimensional numerical model of a spherical explosion tank was developed to explore the effects of water vapor on gas explosions in a high-pressure environment. Explosion parameters of 10% gas, 1 MPa pressure, and water vapor contents varying from 0% to 8% were simulated using FLUENT software. The results show that the maximum explosion pressure and temperature of the premixed gas gradually decrease with increasing water vapor content, i.e., when the water vapor content is increased from 0% to 8%, the maximum explosion pressure and temperature of the gas mixture decreases from 2.52 MPa and 2092 K under dry conditions to 1.62 MPa and 1714 K with 8% water vapor. The attenuation amplitude is also reduced upon the addition of steam. Water vapor in premixed gas therefore plays a vital role in suppressing gas explosions.

Keywords high pressure environment, gas explosion, water vapor, explosion pressure, numerical simulation.

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1 Introduction

Gas explosions have always been the number one threat to safety in coal mines and other industries, especially in high-temperature and high-pressure environments where the hazards and potential damage of gas explosion are more serious (Li et al. 2018). Water exists as steam at high temperatures and pressures, which influences the local humidity and can eventually affect the conditions under which gas explosions occur (Song and Zhang 2019). Gases of a certain humidity are widely present during coalbed methane extraction processes. The water vapor content is often close to saturation and the distribution of corresponding components is more complicated than a simple methane-air mixture, which makes determination of factors that affect explosive properties difficult (Zhang et al. 2018; Pei et al, 2018a). Flooding methods are typically used to extinguish fires in a coal bunker or underground coal pile (Zhou and Guo 2018). Upon entering the high-temperature coal body, however, the water quickly vaporizes and blends with the surrounding gases in the relatively closed environment, which can lead to further explosions and far more serious consequences than the initial explosion (Xu et al. 2016; Pei et al. 2018b). Understanding the effects of water vapor on gas explosions in high-pressure environments is therefore of critical importance.

An underground gas explosion instantaneously generates high temperatures and pressures and, under certain conditions, the environment is likely to experience secondary or even multiple explosions, which are influenced by the high-temperature and high-pressure steam generated by the primary explosion. These issues are addressed in the study of explosion propagation law and gas explosion characteristics. Li et al. (2009) conducted a systematic experimental study on the suppression of methane combustion and explosion by water vapor in an explosion shock tube, and numerically analyzed the mechanism of its anti-combustion and anti-explosion chemical kinetics.

Luo et al. (2008) studied the activation of water vapor and its control on gas explosion using a small self-designed experimental set up. Si et al. (2014) applied flow field simulation software to numerically simulate gas explosions in a high-pressure environment, and analyzed the pressure, temperature, and velocity fields during the explosion process. Lu et al. (1998) analyzed the chemical reaction kinetics of water in gas explosions and explored the relationship between water content and gas explosion intensity through explosion reaction equilibrium. Liang et al. (2017) used chemical reaction kinetic theory and a detailed gas explosion reaction mechanism to analyze the effects of water and CO₂ on gas explosion reaction kinetics in a closed space. Bi et al. (2012) performed experiments to test the effects of water evaporation on a flame surface and during gas explosions, and introduced a mechanism of water suppression. Li et al. (2010) proposed a water curtain suppression system and experimentally demonstrated effective suppression of underground gas explosions under certain conditions. To suppress and isolate gas and coal dust explosion accidents, Fan et al. (2011) developed and tested a water curtain explosion-proof facility. Jia et al. (2013) established a mathematical model of the gas explosion reaction in a confined space to investigate the damping effect of the chemical reaction kinetics of carbon monoxide and water vapor. They found that damped gas explosions with water vapor are superior to those of carbon monoxide. Yu et al. (2015) reported the effects of water mist on the law of gas explosion propagation and regularity based on self-luminous spectral characteristics, which they extended to water mist suppression technology.

The explosive substance is a two-phase (i.e., gas-liquid) mixture and explosion mechanisms involve more complicated factors, such as droplet breaking, vaporization, and heat absorption. Water vapor always exists in the natural environment (Liu et al. 2003). If the water vapor in the premixed

gas is unsaturated, it can be assigned to a typical pure gas phase explosion problem, which can be studied by gas explosion correlation analysis methods. Current studies have mainly addressed gas explosion and gas mist suppression in a high-temperature environment. However, only a few studies have examined the effect of water vapor on gas explosion characteristics in a high-pressure environment.

In this study, a two-dimensional numerical model was developed based on a spherical explosion tank. The EBU (Eddy breakup) model of FLUENT software was applied to simulate explosion characteristics under high-pressure conditions and variable premixed steam-gas content. The results are used to quantitatively explore the inhibition effects of water vapor content on gas explosions.

2 Mathematical models and conditions

2.1 Mathematical models and calculation methods

2.1.1 Control equations

(1) Mass conservation

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{u}) = 0 \quad (1)$$

where ρ represents density, div is divergence, t is time, and \vec{u} is the velocity vector.

(2) Momentum conservation

$$\frac{\partial(\rho T)}{\partial t} + \text{div}(\rho \vec{u} \vec{u}) = \text{div}(\mu \text{grad} \vec{u}) - \frac{Dp}{Dt} + S_u \quad (2)$$

where p is the fluid micro-body pressure, μ is the dynamic viscosity, and S_u is the generalized original term of the momentum conservation equation.

(3) Energy conservation

$$\frac{\partial(\rho T)}{\partial t} + \text{div}(\rho \vec{u} T) = \text{div}\left(\frac{k}{c_p} \text{grad} T\right) + S_T \quad (3)$$

where c_p is the specific heat capacity, T is temperature, k is the fluid heat transfer coefficient,

and S_T is viscous dissipation.

(4) Component transmission

$$\frac{\partial}{\partial t}(\rho Y_i) + \text{div}(\rho \vec{u} Y_i) = \text{div} \vec{J}_i + R_i + S_i \quad (4)$$

where Y_i is the volume concentration of component i , R_i is the net rate of the chemical reaction, S_i is the additional generation rate due to discrete phase and user-defined source terms, and J_i is the diffusion flux of substance i . The diffusion flux \vec{J}_i can be expressed as:

$$\vec{J}_i = \rho D_{i,m} \text{div} Y_i \quad (5)$$

where $D_{i,m}$ is the diffusion coefficient of substance i in the mixture.

$$\vec{J}_i = \rho D_{i,m} + \frac{\mu_t}{Sc_t} \text{div} Y_i \quad (6)$$

where Sc_t is the turbulent Schmidt number, and $\frac{\mu_t}{\rho D_t} = 0.7$.

(5) Turbulence equation

In this paper, the standard k- ϵ turbulence model widely used in engineering is applied for the turbulence of the flame:

$$\rho \frac{Dk}{Dt} = \frac{\partial}{\partial x_i} \left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} + G_k + G_b - \rho \epsilon - Y_M \quad (7)$$

$$\rho \frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_i} \left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial \epsilon}{\partial x_i} + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} \quad (8)$$

where G_k indicates the turbulent flow energy generated by the average velocity gradient, G_b represents the turbulent energy caused by buoyancy, and Y_M is the effect of compressible turbulent pulsation expansion on the total dissipation rate. The turbulent viscosity coefficient can be expressed as:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (9)$$

In FLUENT, default value constants, $C_{1\epsilon} = 1.44$, $C_{2\epsilon} = 1.92$, $C_u = 0.09$, are used, and the

turbulent Prandtl number of the turbulent flow energy k and dissipation rate ε are set to $\sigma_k = 1.0$ and $\sigma_\varepsilon = 1.3$ respectively.

(6) Ideal gas state equation

$$p = \rho RT \quad (10)$$

where R is the molar gas constant.

2.1.2 .Calculation methods

The conservation equations established in the above mathematical model can be expressed as:

$$\frac{\partial(\rho\varphi)}{\partial t} + \text{div}(\rho \vec{u} \varphi) = \text{div}(\Gamma \text{grad}\varphi) + S \quad (11)$$

where φ is the general variable, $\frac{\partial(\rho\varphi)}{\partial t}$ is the unsteady term, $\text{div}(\rho \vec{u} \varphi)$ is the convection term, $\text{div}(\Gamma \text{grad}\varphi)$ is the diffusion term, and S is the original item.

The finite volume method is applied to deal with the governing conservation equations. The partial differential equations are integrated into the control body and converted into discrete variables, and the algebraic equations are linearized.

The instable term discretization adopts the Gauss-Seidel first-order implicit scheme, the convection term discretization adopts the first-order upwind style, the divergence term adopts the central difference scheme, and the source term adopts linearization processing. In this paper, eqn (9) is discretized by the PISO algorithm. CFD (Computational fluid dynamics) software is used to solve the discrete equations of the basic governing equations, the pressure-based transient solver is used, and the pressure-velocity coupling equation is solved by the SIMPLE algorithm. The gradient difference is in the GREEN-GAUSS node-based format and the remaining spatial quantities (including pressure, density, momentum, turbulence variables, and the scalar components of combustion components) in addition to time differences are all second-order up-style. The unclosed

term that occurs after the equation is discretized must be closed by a mathematical model that includes the turbulence model, the chemical reaction model, and the wall function at the near wall. Considering various factors, the RNG k- ϵ model is selected as the turbulence model, and the combustion model is a general finite-rate model. The near-wall area is simulated using the unbalanced wall function method, and appropriate mesh encryption is performed at the wall.

2.2 Numerical model

The geometric model of the near spherical container is shown in Fig. 1(a). Symmetry methods are applied for modeling because the explosion tank is symmetrical about the central axis. The material is stainless steel and the interior contains a mixture of gas, water mist, and air. The grid model is shown in Fig. 1b. The calculation area is divided by the grid structure, which is centered at 0.2 mm.

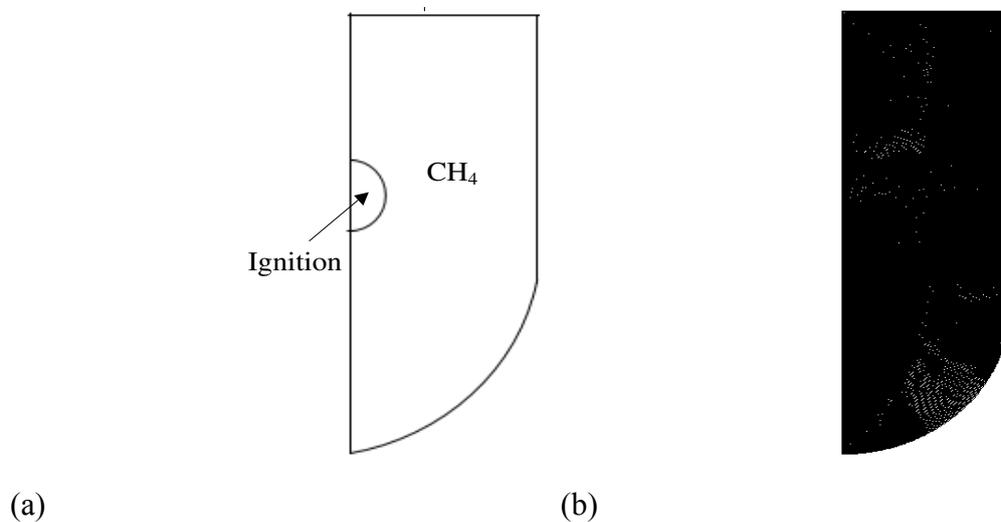


Fig. 1 Schematic diagram of a nearly spherical model: (a) 1/2 physical model; (b) 1/2 grid model.

2.3 Initial conditions, boundary conditions, and related assumptions

2.3.1 Initial conditions

Let the initial time be t_0 , then $T(t_0) = T_0$, $p(t_0) = p$, and $u(t_0) = 0$. The internal premixed gas is

mainly 10 vol.% gas-air-steam, such that

$$m(CH_4)(t_0) = 0.054(1 - x), \quad m(O_2)(t_0) = 0.22(1 - x), \quad m(H_2O)(t_0) = x, \quad m(CO_2)(t_0) = 0$$

2.3.2. Boundary conditions and ignition conditions

The adopted boundary conditions are adiabatic wall surfaces. Symmetrical boundary conditions are used for a simplified calculation because the container is a symmetrical structure. The ignition process of industrial gases can be explained by thermal explosion theory. First, the ignition source generates energy to heat the local combustible gas near the fire source causing the temperature to rise rapidly, and ignition occurs upon reaching the ignition temperature. Second, the flammable gas spreads by propagation of the flame to cause ignition of the entire combustible gas-air premixed system. Therefore, according to the theory of thermal ignition, the mass of high-temperature burned gas can be set in the ignition zone of the simulation calculation. The temperature and concentration of the burned gas are follows:

$$T(t_0) = 1500 \text{ K}, \quad p(t_0) = 1 \text{ MPa}, \quad u(t_0) = 0, \quad m(CH_4)(t_0) = 0, \quad m(O_2)(t_0) = 0$$

$$m(H_2O)(t_0) = x, \quad m(CO_2)(t_0) = 0.001$$

2.3.3. Related assumptions

- (1) The water mist ignores the macroscopic state of different particle sizes, and the complex phase transition process (e.g., steam evaporation) is simplified by changing the thermal properties;
- (2) Irradiation heat transfer is not considered;
- (3) Influence of the volume force is ignored;
- (4) Viscous dissipation is zero, excluding the Soret effect and Dufour effect.

This study investigated the effect of water vapor content on gas explosions. In the numerical simulations, 10% gas-air was combined with water vapor contents of 0%, 2%, 4%, 6%, and 8% in a

high-pressure environment, and the pressure, temperature, and speed during the simulation were monitored.

3 Results and discussion

3.1 Effect of water vapor content on gas explosion pressure

Fig. 2 shows the effect of explosion pressure on CH₄-O₂ mixed gas with different water vapor contents in a high-pressure environment. As water vapor content increases, the gas pressure and maximum explosion pressure during the explosion development decreases. For example, the maximum explosion pressure decreases from 2.52 to 1.62 MPa when the water vapor content increases from 0% to 8%. The rate of pressure change with respect to time also decreases significantly.

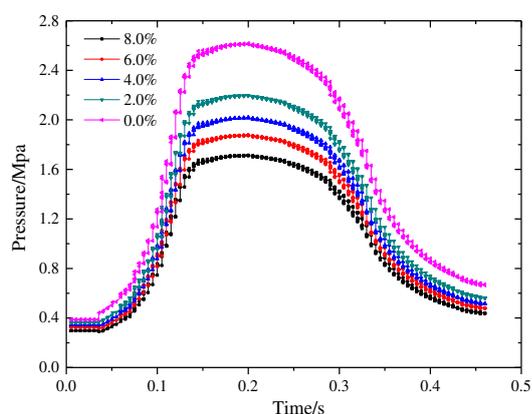


Fig.2 Explosion pressure of premixed gas-steam as a function of time using different water vapor contents.

The variation trends of the maximum explosion pressure under different explosion limits of water vapor are proportionally scaled. Except for the maximum pressure rise in Fig. 2, the maximum explosion pressure after the addition of water vapor is greatly reduced. The increase of inert water vapor content increases the stoichiometric ratio of the fuel and oxidant, while the water vapor content of the premixed gas in the simulation remains unsaturated. The main components are still methane

and air but the water vapor content is relatively low (volume fraction is less than 10%), and the explosive suppression capacity is relatively limited. When the methane is near the optimal explosion concentration, the explosion is in a “strong” state. Furthermore, the mixing of a small amount of water vapor causes a fuel/oxidant imbalance of the reaction system, further hindering the development of the explosion, and resulting in a relative decrease in the maximum explosion pressure.

3.2 Effect of water vapor content on gas explosion temperature

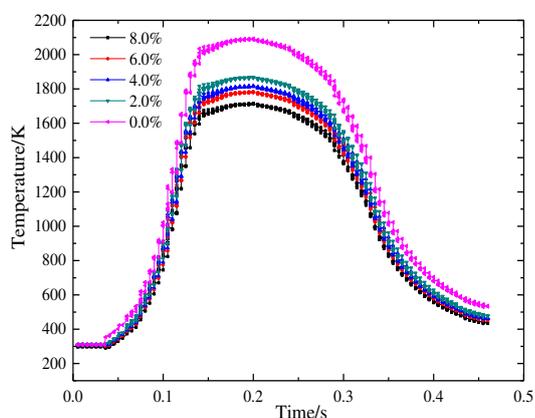


Fig. 3 Explosion temperature of premixed gas-steam as a function of time using different water vapor contents.

Fig. 3 shows the variation of explosion temperature of the $\text{CH}_4\text{-O}_2$ mixed gas with different water vapor concentrations. The maximum temperature in the container is maintained between 1500 and 3000 K. When the ignition temperature and ambient pressure are constant, the maximum temperature of the system explosion reaches 2902 K when no steam is added. As the water vapor content increases, the maximum temperature gradually decreases, with an average reduction of 94.5 K. According to **Fig. 3**, the entire explosion process can be divided into three stages:

(1) Explosion initial stage. During this stage, the temperature in the vessel rises slowly and, as the water vapor content increases, the period gradually increases. The explosion reaction emits a

large amount of heat that is continuously conducted to the surroundings, causing the center temperature to drop. Because there are many reactants in the container, some of the heat energy is consumed during the chemical reaction. The released heat energy is greater than the consumed heat energy so the temperature tends to slowly rise.

(2) Explosion expansion phase. The temperature rises rapidly during this stage. The heating rate gradually decreases with increasing water content. Because the numerical simulation is an adiabatic process, fewer reactants remain as the explosion reaction proceeds and the heat absorbed by the reaction is reduced. Heat is continuously released during the reaction, which causes the temperature to rapidly rise. At this point, the flame reaches the wall and is distorted. Energy released by the reaction tends to equal the cooling effect of the water vapor and energy consumed by the leakage, so that the explosion pressure tends to maximize.

(3) Explosion decay phase. During this stage, heat transfer in the vessel has almost ended, the temperature tends to stabilize, and the reaction is nearly complete. Energy loss in a real experiment causes a reduction of both pressure and temperature because the generated reaction energy is less than the energy loss.

3.3 Effect of water vapor content on gas explosion velocity

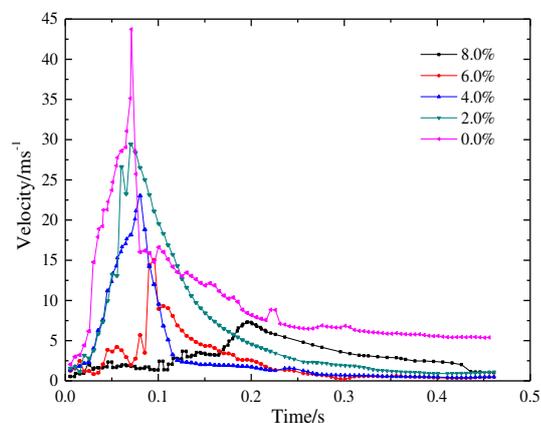


Fig. 4 Explosion velocity of premixed gas-steam as a function of time

using different water vapor contents.

The five explosion velocity curves show similar trends for all compositions studied (Fig. 4). The curves gradually increase at the beginning of the explosion. The burning speed is rapid under high pressure, and the increase of the burning speed is clear before the release of ignition energy and formation of a stable combustion flame surface. However, the peak velocity gradually decreases with increasing water vapor content. The burning rate of the gas flame surface is further reduced due to the encapsulation of water vapor, leading to a physical decline process. The burning speeds of the five different compositions are basically the same in the later stages of the explosion, and velocities are essentially balanced after 0.4 s. The flame speed reaches 5 m/s when no steam is added, and reduces to 2.5 m/s upon the addition of 8% steam.

3.4 Water vapor suppression

When a gas explosion occurs, the shock wave generated by the explosion causes an increase in the ambient temperature and pressure, providing a high-temperature and high-pressure environment for a secondary explosion. This leads to an increase in the intramolecular energy and number of activated molecules in the new system, resulting in an increase in the frequency of collisions between molecules and production of more chain reaction free radicals. In addition, the chemical chain reaction is easier to carry out, which makes the original system more flammable and explosive. To some extent, high initial pressures also enhance the participation of methane gas in the explosion reaction, resulting in an increase of the chemical reaction rate and yielding a more active system at the critical explosion point.

When water vapor is added to the gas-air mixture, the concentration of reactants decreases, causing weakened molecular motion and reduced dissociation of high-activity radicals. The gas

explosion intensity is thereby reduced and can even be inhibited. Moreover, because of the large specific heat of water vapor, a heat exchange effect occurs with a large number of surrounding water molecules, which reduces the pressure, temperature, and speed of the mixed with the addition of water vapor. It is worth noting that the suppression of gas by water vapor is a pure gas phase explosion problem. The action mechanism is based on the fact that water vapor molecules act as an inert medium and hinder the progress of chemical reactions, which is a key factor in water mist suppression. In addition, the water molecule content in the explosion system is much lower than that when water vapor is suppressed. Under natural environmental conditions, unsaturated water vapor only weakens the pressure of the explosion process and cannot completely inhibit its development. Relevant analytical methods can be extended to analyze inhibition effects in a multi-phase explosion problem when saturation is exceeded or when droplets precipitate.

4 Conclusions

(1) We explored the effects of water content on gas explosions under an ignition pressure of 1 MPa and ignition temperature of 1500 K. As water vapor content increases from 0% to 8%, the gas explosion time gradually increases, and the gas pressure, maximum explosion pressure, and rate of pressure change all decrease. When the water vapor content is reduced from 8% to 0%, the maximum explosion pressure increases from 1.62 to 2.52 MPa, while the maximum pressure time increases gradually.

(2) The pressure and temperature characteristics in the explosion limit exhibit a parabolic distribution. The maximum explosion pressure and temperature of the gas mixture decreases from 2.52 MPa and 2092 K under dry conditions to 1.62 MPa and 1714 K with 8% water vapor. The maximum pressure is affected by the ambient humidity far beyond the maximum temperature.

(3) At the beginning of the explosion, the curve of explosion velocity versus time shows a gradual upward trend with a rapid burning speed under high pressure. The peak velocity gradually decreases as the amount of water vapor increases. However, during the later explosion stage, the burning speeds were essentially the same regardless of the composition. Speed values stabilized after 0.4 s.

(4) In a high-temperature and high-pressure environment, the mixing of water vapor can delay the chemical reaction between methane and air, reducing the gas explosion pressure and heat convection characteristics and suppressing the gas explosion.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

- Bi MS, Li Z, Zhang PP (2012) Experimental study on water mist suppressing gas explosion. *Journal of Mining and Safety Engineering* 29(3): 440–443.
- Fan XT, Li RZ, Xue SQ (2011) Experimental study on explosion-proof effect of water curtain in coal mine gas explosion. *Mining Safety and Environmental Protection* 38(2): 17–19.
- Jia BS, Wang XY, Zhang SY (2013) Study on water curtain system of explosion suppression for coal mine gas explosion. *Fire Safety Science*, 22(3): 131–139.
- Liang YT, Wang LC, Luo HZ, Feng EB (2017) The kinetic calculation model of shock-induced gas explosion reaction. *Journal of China Coal Society* 42(6): 1475–1481.
- Li CB, Wu GD, Jing FQ (2009) Experimental investigation and numerical computation of methane combustion and explosion suppressed by vapor. *China Safety Science Journal* 19(1): 118–121.
- Li RZ, Si RJ, Gao K, Qin XX, Wen LX (2018) Experimental study on the effect of explosion suppression in low-concentration gas transportation. *Journal of Loss Prevention in the Process Industries* 54: 216–221.
- Li RZ, Si RJ, Xue SQ (2010) Study on water curtain system of explosion suppression for coal mine gas explosion. *Coal Technology* 29(3): 102–104.
- Liu HY, Lu SX, Qin J (2003) Experimental study on inhibiting the gas explosion flame by water spray. *China Safety Science Journal* 13(8): 74–80.
- Lu SX, He J, Yu CH (1998) Mechanism of gas explosion suppression by water. *Journal of China Coal Society* 23(4): 417–421.
- Luo ZM (2008) Experiment study on controlling gas explosion by active steam. *Coal Geology & Explosion* 36(3): 23–26.

- Pei B, Wei SM, Yu MG, Chen LW, Pan RK, Wang Y, Li J, Jing GX (2018b) Synergistic effect of gas-liquid two-phase medium to suppress pipeline methane explosion. *Journal of China Coal Society* 43(11): 184–190.
- Pei B, Yang Y, Li J, Yu MG. (2018a) Experimental study on suppression effect of inert gas two fluid water mist system on methane explosion. *Procedia Engineering* 211: 565–574.
- Si RJ (2014) Numerical simulation of gas explosion characteristics under high pressure environment. *Coal Mine Safety* 45(7): 1–4.
- Song YF, Zhang Q (2019) Quantitative research on gas explosion inhibition by water mist. *Journal of Hazardous Materials* 363–16
- Xu YL, Wang LY, Yu MG, Wan SJ, Song ZP, Wang SK (2016) Study on the characteristics of gas explosion affected by induction charged water mist in confined space. *Journal of Loss Prevention in the Process Industries* 40: 227–233.
- Yu MG, Zhu XN, Pei B, Yang Y (2015) Experimental Study on CO₂-Ultrafine Water Mist for Inhibiting Methane Explosion. *Journal of China Coal Society* 40(12): 101–106.
- Zhang JJ, Cliff D, Xu KL, You G (2018) Focusing on the patterns and characteristics of extraordinarily severe gas explosion accidents in Chinese coal mines. *Process Safety and Environmental Protection* 117: 390–398.
- Zhou XH, Guo K (2018) Experimental Study on Suppression of Gas Explosion by Explosion Proof Water Curtain. *Mining Safety and Environmental Protection* 45(4): 44–48.

Figures

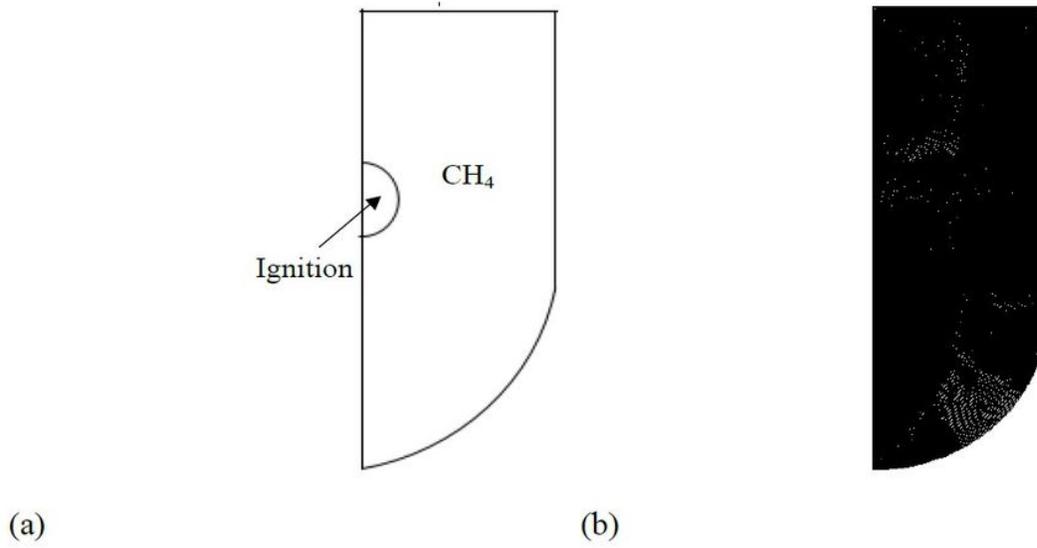


Figure 1

Schematic diagram of a nearly spherical model: (a) 1/2 physical model; (b) 1/2 grid model.

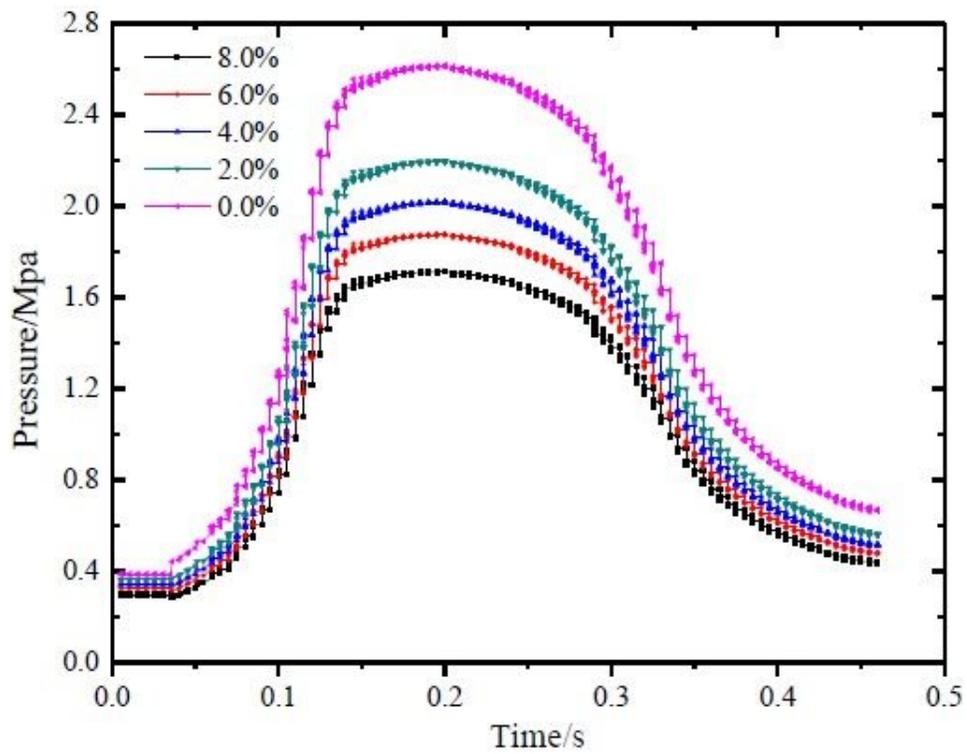


Figure 2

Explosion pressure of premixed gas-steam as a function of time using different water vapor contents.

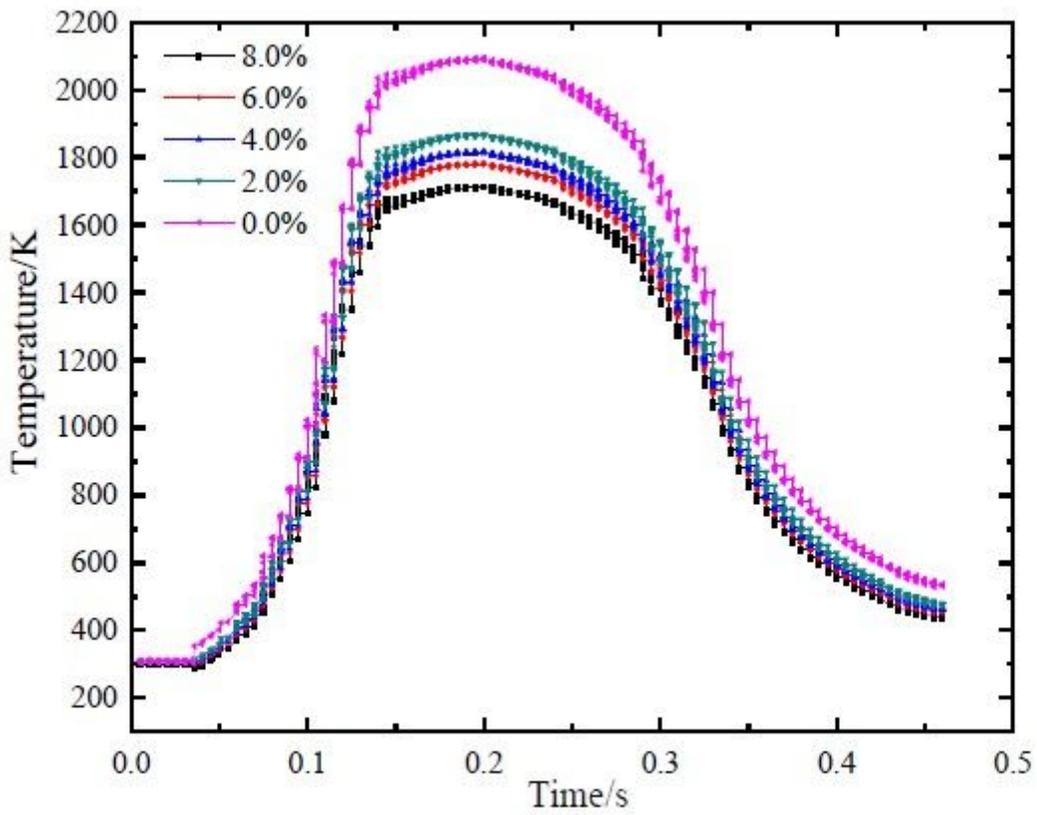


Figure 3

Explosion temperature of premixed gas-steam as a function of time using different water vapor contents.

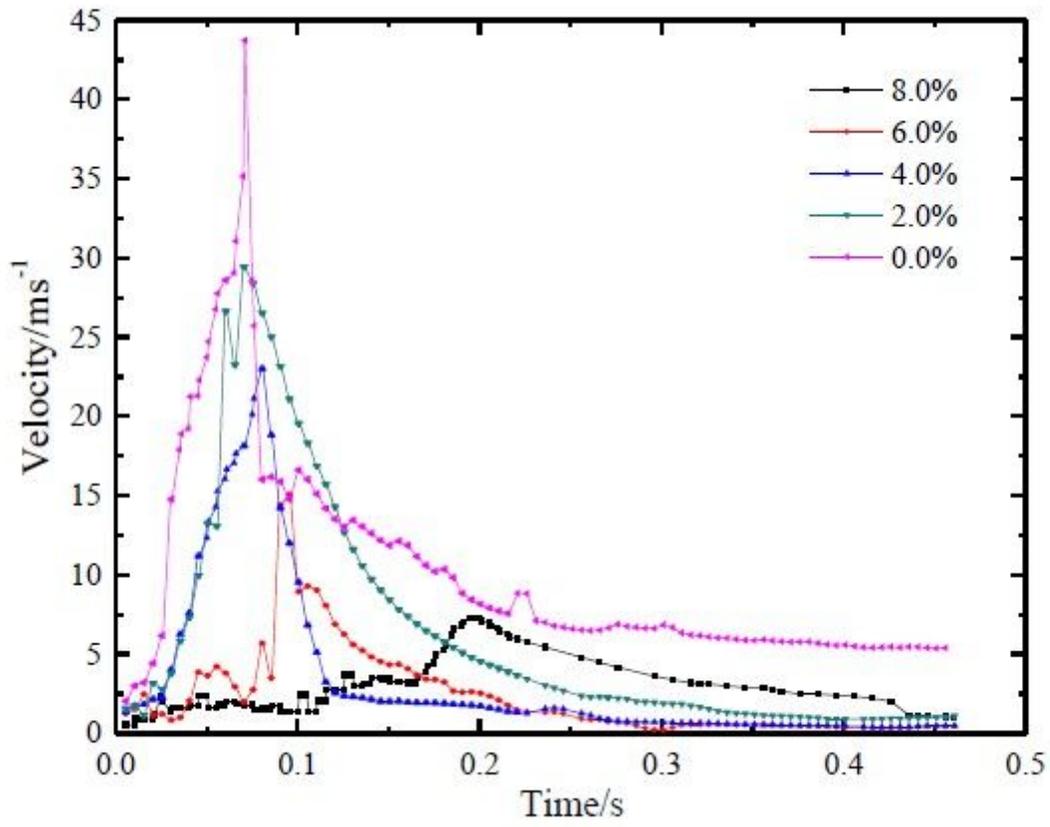


Figure 4

Explosion velocity of premixed gas-steam as a function of time