Numerical simulation of the inhibition process of methane-air explosion under cold aerosol

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Abstract. In order to study the methane-air explosion suppression problem, a certain size experimental tube was used as the physical model, and Gambit was used for modelling. The ANSYS 15.0 software was used to simulate the methane-air explosion suppression process under the action of cold aerosol, and the simulation results were compared with the results of the experimental studies in the open literature. It can be seen from the numerical simulation results that the concentration of cold aerosol had a significant effect on the methane-air explosion process. When the concentration of cold aerosol was low, the methane-air would explode. The pressure-time curve in the experimental tube showed four stages: the explosion induction period, the pressure rise phase, the explosion pressure peak value phase and the explosion pressure decay phase. With the increase of the aerosol concentration, the explosion induction period was significantly prolonged, and the maximum explosion pressure was slightly decreased, and the time to reach the maximum explosion pressure was also significantly prolonged. When the cold aerosol concentration reached a certain threshold, the methane-air no longer exploded. Compared with the experimental results, the simulated values of the explosion induction period, the maximum explosion pressure value, the maximum explosion pressure time and the final pressure value under different cold aerosol concentrations matched well with the experimental measurements. Therefore, numerical simulation can provide a reference for the study of methane-air explosion suppression performance under cold aerosol.

1. Introduction
The prevention and suppression of gas-air (especially methane-air) mixture explosions has been a very important and cumbersome problem because they are the main cause of frequent casualties and economic losses in coal mines.

Gas explosion is a very complex process, which involves the multiphase coupling and intersection of physical processes, chemical processes, thermodynamic processes, heat and mass transfer processes, etc. The principles of suppressing gas explosion mainly include cooling, inertization, termination reaction, barrier and quenching [1]. According to various mechanisms preventing combustion explosion and diffusion, there are many anti-explosion technologies involved, such as high-pressure water curtain, nitrogen curtain, rock powder shed, water bag, dry powder fire extinguishing agent, N2/CO2 mixture, ultra-fine water mist-porous material, quenching by fire barrier, N2-two-fluid water mist containing NaCl additive, aerosol fire extinguishing agent. [2-5] Among them, aerosol fire extinguishing agent is a...
new type of fire extinguishing agent, which has many advantages of green environmental protection, high speed of fire extinguishing, low price, wide fire extinguishing range, zero ozone depletion potential (ODP), low global warming potential (GWP), no poisoning, etc. Therefore, it has a broad application prospects in many fields, such as mines, subway tunnels, cable trenches. [6-9] Aerosol fire extinguishing agents are classified into cold aerosols and hot aerosols fire extinguishing agents. The fire extinguishing mechanism of the former is to achieve the purpose of fire extinguishing by the chemical inhibition of solid particulate components in the unit mass in a confined space, wherein the smaller particles ensure their residence time in space, effectively react with the active substances in the flame inhibiting combustion, and larger particles ensure that they can have enough momentum and density to pass through the flame to quickly extinguish the fire. The latter's fire-extinguishing mechanism is mainly based on the chemical inhibition of solid particulate components per unit mass in a confined space. The inert gas component dilutes oxygen as a supplement to achieve fire extinguishing. In other words, the fire is extinguished by methods of endothermic decomposition and cooling, chemical inhibition of gas phase and solid phase, and inert gas dilution of oxygen. In general, aerosol fire extinguishing agents extinguish fires by the synergistic effect of cooling, dilution and chemical inhibition [10]. In addition, its excellent fire extinguishing performance is also attributed to its dynamic behavior. In the process of fire extinguishing, the dynamic behavior of aerosol fire extinguishing agent is as follows. First, aerosol has a good flow performance, and it can bypass obstacles to reach the protection zone with a full flooding effect. Second, besides the role of driven gas, aerosol is also subjected to other forces, such as airflow resistance, mass force, buoyancy, pressure gradient force and Staffman lift, so it has the ability to suspend steadily during the fire extinguishing process. Finally, solid particulates constantly exchange momentum and energy with the gas phase and collide with the wall, so constantly change their motion speed and direction [11]. The above kinetic behavior of aerosol fire extinguishing agents gives it excellent suppress explosion properties, which has been confirmed by experiments [12, 13].

At present, there are several studies on the suppression of methane-air combustion explosion with aerosol fire extinguishing agent as the anti-explosive agent. Among these, the experimental research is the majority [12, 13] and the related numerical simulation research is few. The author first established the same proportion of the three-dimensional physical model used in the literature [14], and then used ANSYS 15.0 software [15] to simulate the inhibition of aerosol on 10% methane-air mixture explosion to quantitatively analyze the variation of pressure on the explosion suppression characteristics. The above obtained results were compared with the experimental results in [14]. The study is hopefully believed to provide a basis for studying the inhibition characteristics of gas explosion.

2. Numerical Simulation
Krasnyansky [14] had studied the inhibition of aerosols on 10% methane-air mixture explosion. The specific steps were as follows. First, the pressure in the experimental device (a closed tube with a diameter of 0.1 m and a length of 1.5 m) was reduced to $1.1 \times 10^3$ Pa. Then, the 10% methane-air mixture was introduced from the inlet shown in figure 1. The test tube was ignited simultaneously passing through the aerosol (its composition consisted of solid particulates and inert gases), and the variation of pressure in the experimental apparatus was experimentally studied. The solid compositions in the aerosol included 78% (in mass) urea, 20% (in mass) potassium chloride and 2% (in mass) silica. The gas in the aerosol was a complex of nitrogen, carbon dioxide and water vapor, etc. The test parameters in numerical simulation was set according to Krasnyansky’s [14]. The obtained results were compared with the experimental results. The physical model of the experimental device and the pressure measurement point were shown in figure 1.
Figure 1. The geometric model of an experimental setup

As shown in figure 2, the grid unit used a structured hexahedral mesh, and the mesh near the aerosol and methane-air vents was densified.

Figure 2. The grid model of an experimental setup

In order to reduce the influence of the grid structure on the calculation accuracy, the grid parameters were optimized referring to the CFD software’s optimization parameters which were used to build the gas explosion model [16]. The sensitivity of several different grid structures were analyzed, as shown in table 1. Clearly, the grid scheme 2 was the optimal one, which obtained relatively accurate calculation results.

| No. | The grid scheme | Quantity | Maximum pressure error | Wall stress error |
|-----|-----------------|----------|------------------------|-----------------|
| 1   | 2000×2000       | 4000000  | 0.013%                 | 0.019%          |
| 2   | 1500×1500       | 2250000  | 0.028%                 | 0.031%          |
| 3   | 1200×1200       | 1440000  | 0.067%                 | 0.07%           |
| 4   | 900×900         | 810000   | 0.104%                 | 0.091%          |

The Euler-Lagrangian method was used to simulate aerosol-jet two-phase flow. The fluid and particles were treated as a continuous medium and a discrete phase, respectively [17-19]. There was a coupling between the discrete phase and the continuous phase. The Staffman lift of the discrete phase due to shearing was considered. For discrete phases, non-steady-state tracking was chosen. The particles were inert, nonreactive. The particles had an average diameter of 30-40 μm. The initial temperature of the particle flow was 300 K. Consider to the effect of turbulence on the particles, the survival time of the turbulent vortex was determined to be constant.

3. Simulation results and analysis

Figure 3 shows the curves of pressure versus time at various concentrations of aerosol. As can be seen from figure 3, there was an aerosol concentration threshold for the suppression of methane-air explosion. When the concentration of the aerosol was less than 10.1 g/m$^3$ or without aerosol, the explosion of methane-air happened. When the concentration of aerosol reached 10.1 g/m$^3$, methane-air no longer exploded. When explosion happened, the pressure-time curve could be divided into four stages, namely, the explosion induction period, the pressure rise stage, maximum pressure stage and stage of decay of explosion pressure.

When the concentration of the aerosol was 0 g/m$^3$, the pressure-time curve exhibited a four-stage trend (see figure 3a). Specifically, the initial pressure was stable at 0.210×10$^5$ Pa and the corresponding
explosion induction duration was 0.108 s. Then, the pressure rapidly increased and reached to the maximum explosion pressure value \((3.278 \times 10^5 \text{ Pa})\) at 0.482 s. Thereafter, the pressure showed a trend of a significant drop followed by a slow decrease, and the final pressure was stable at \(0.386 \times 10^5 \text{ Pa}\).

When the concentration of the aerosol was 2.9 g/m\(^3\), the pressure-time curve also showed a four-stage trend (see figure 3b). Specifically, the initial pressure was maintained at \(0.210 \times 10^5 \text{ Pa}\) and the corresponding explosion induction duration was 0.210 s. Then, the pressure increased continuously and reached the maximum explosion pressure value \((3.281 \times 10^5 \text{ Pa})\) at 0.791 s. Subsequently, the pressure gradually decreased and the final pressure stabilized at \(0.172 \times 10^5 \text{ Pa}\). In comparison, the explosion induction period in figure 3b was 1.94 times of that in figure 3a, which was mainly due to the introduction of aerosols in the methane-air mixture [12]. With the introduction of a certain amount of aerosol, the solid particles and inert gas contained in the aerosol absorbed the heat released by the methane-air explosion at the moment of ignition, and the flame temperature was lowered. Thus, the heat radiated to the surface of the methane-air combustion was reduced and the amount of free radicals produced by the methane-air explosion also decreased. At the same time, the cation generated by the gasification of the solid particles instantaneously reacted with the active groups (such as \(\cdot \text{H}, \cdot \text{OH} \text{ and } \cdot \text{O}\)) in the combustion, thereby achieving the purpose of suppressing the exothermic reaction between the radicals. Aerosol particles had a large specific surface area and were capable of adsorbing chain reaction propagators, including \(\cdot \text{H}, \cdot \text{OH} \text{ and } \cdot \text{O}\). Therefore, the heat loss in the methane-air explosion reaction increased, prolonged the explosion induction period and the duration of reaching the maximum explosion pressure. Since the concentration of the aerosol in figure 3b was not sufficient to suppress the methane-air explosion, its maximum explosion pressure was very similar to that of figure 3a.

![Figure 3. Pressure-time curves of methane-air mixtures with aerosol of different concentrations. The aerosol concentrations in figures a-e are 0, 2.9, 5.6, 8.5 and 10.1 g/m\(^3\), respectively.](image-url)
When the concentration of the aerosol introduced was 5.6 g/m$^3$, the pressure-time curve also showed a four-stage trend (see figure 3c). Specifically, the pressure was maintained at 0.210$\times$10$^5$ Pa and the corresponding explosion induction duration was 0.352 s. The pressure increased continuously and reached the maximum explosion pressure value (3.269$\times$10$^5$ Pa) at 0.898 s. Subsequently, the pressure gradually decreased and the final pressure stabilized at 0.384$\times$10$^5$ Pa. The explosion induction period in figure 3c was 3.24 times of that in figure 3a. The reason was mainly related to the introduction of aerosols, which had been explained above. In addition, the maximum explosion pressure value in figure 3c was similar to that in figures 3a and 3b, because the concentration of aerosol was not sufficient to inhibit methane-air explosion.

When the concentration of the aerosol introduced was 8.5 g/m$^3$, the pressure-time curve also showed a four-stage trend (see figure 3d). Specifically, the pressure was maintained at 0.210$\times$10$^5$ Pa and the corresponding explosion induction duration was 0.761 s. The pressure increased continuously and reached the maximum explosion pressure value (3.262$\times$10$^5$ Pa) at 1.344 s. Subsequently, the pressure gradually decreased and the final pressure stabilized at 0.288$\times$10$^5$ Pa. In comparison, the explosion induction period in figure 3d was 7.04 times of that in figure 3a. The reason was mainly related to the introduction of aerosols. The specific reasons had been elaborated above and would not be described here. In addition, the maximum explosion pressure value in figure 3d was similar to that of figures 3a, 3b and 3c, which was primarily related to the concentration of aerosol not sufficient to inhibit methane-air explosion.

When the concentration of aerosol introduced was 10.1 g/m$^3$, the pressure-time curve in figure 3e exhibited a different trend from figures 3a-3d. Specifically, the initial pressure in figure 3e was maintained at 0.210$\times$10$^5$ Pa and the corresponding explosion induction duration was 0.700 s. Then the pressure was gradually lowered and the final pressure was stable at 0.076$\times$10$^5$ Pa. The maximum explosion pressure did not appear in figure 3e. So it was concluded that the methane-air explosion was suppressed. The reasons mainly included the following three aspects [12]. First, when a sufficient amount of aerosol was introduced, the concentration of methane was lowered, which was insufficient to generate enough free radicals (such as $\cdot$H and $\cdot$CH$_3$), thereby reducing the number of chain reactions and then the oxidation rate of methane. Therefore, the explosive reaction was not easy to occur. Second, modern combustion theory [20] believed that most combustion reactions occurred when collisions occurred among reactive reactant molecules. When molecular collision happened, the factors including form, energy and angle would affect the effective of the collisions, then the reaction rate. The addition of an aerosol to methane-air enhanced the three-body reaction in the gas explosion reaction mechanism. The aerosol acted as a third body and participated in the ternary collision in the chain reaction. Under the high explosion pressure, the ternary collision frequency was higher than the binary collision frequency, which greatly reduced the concentration of the activation centre of the branch reaction, and transferred the energy of a large amount of free radicals to the inert gas molecules and aerosol solid particles. Therefore, the energy was significantly reduced and the spread of the explosion was suppressed. Finally, the cations which were decomposed by the solid particles in the aerosol inhibited the exothermic reaction between the active groups, interrupted the chain reaction, and consumed the active radicals participating in burning. In addition, the particles adsorbing the pyrolysis product of the combustible substances were not gasified, so that the low molecular product of the combustible material cracking was no longer involved in the reaction of generating the active radical group. Thus, the generation of free radicals was reduced, thereby suppressing the burning rate and the methane-air explosion was completely suppressed.

From the results mentioned above, it could be concluded that the inhibition behavior of the aerosol fire extinguishing agent on the methane-air mixture explosion was mainly related to the aerosol concentration. When the concentration of the aerosol was below a certain concentration threshold (10.1 g/m$^3$), the explosion of the methane-air mixture could not be prevented, and thus the maximum explosion pressure peak occurred (as shown in figures 3a-3d). When the concentration of the aerosol was equal to or higher than this concentration threshold, the methane-air explosion could be prevented. On the one hand, when aerosol particles encountered high temperature, a strong endothermic decomposition
reaction could occur, and the flame temperature was rapidly reduced. On the other hand, the aerosol absorbed the heat radiation of the flame, preventing the thermal feedback between the flame and the combustion product, inhibiting the combustion process. In addition, the aerosol particles and the ions generated by the thermal decomposition of the aerosol particles neutralized with the active radicals generated by the decomposition of combustibles during combustion, thereby blocking the energy transfer during the combustion process and the combustion reaction was suppressed. Finally, the combination of diffusion, Brownian motion, wall reflection and sedimentation of aerosol particles made it possible for particles to reach the combustion position of the methane-air mixture timely to extinguish and the explosion was prevented. Thus, the maximum explosion pressure did not appear in figure 3e.

4. Comparative analysis of numerical simulation and experimental results

The comparisons of the explosion characteristic parameters at different aerosol concentrations obtained in numerical simulations and experiments were shown in table 2.

Table 2. Simulated and experimental explosion characteristic parameter variation in different aerosol concentrations

| Explosion characteristic parameter | Aerosol concentrations, g/m³ | 0    | 2.9  | 5.6  | 8.5  | 10.1 |
|-----------------------------------|-----------------------------|------|------|------|------|------|
| Explosion induction period, s     | Measurement value a         | 0.131| 0.268| 0.363| 0.732| -    |
|                                   | Simulation value             | 0.108| 0.211| 0.352| 0.761| -    |
| Maximum explosion pressure, ×10⁵ Pa | Measurement value a         | 3.286| 3.238| 3.286| 2.857| -    |
|                                   | Simulation value             | 3.278| 3.281| 3.269| 3.262| -    |
| Time to reach maximum pressure, s | Measurement value a         | 0.491| 0.792| 0.893| 1.339| -    |
|                                   | Simulation value             | 0.482| 0.791| 0.898| 1.344| -    |
| Final pressure, ×10⁵ Pa           | Measurement value a         | 0.381| 0.171| 0.381| 0.286| 0.076|
|                                   | Simulation value             | 0.386| 0.172| 0.384| 0.288| 0.076|

Note: The superscript ‘a’ in table 2 indicates that all measurements listed are from the literature [14]. In addition, the ‘-’ in table 2 indicates that it does not explode.

It could be seen from table 2 that when the concentration of aerosol was less than 10.1 g/m³, the simulated value of the explosion induction period increased with the increase of aerosol concentration, which was consistent with the trend of the experimental value. When the aerosol concentration reached 10.1 g/m³, the methane-air no longer exploded, and the results of the simulated and experimental values were also consistent. In addition, when the concentration of aerosol was less than 8.5 g/m³, the simulated values of the explosion induction period were smaller than the measured values. When the aerosol concentration was 8.5 g/m³, the simulated value of the explosion induction period was larger than the experimental value. These might be related to the accuracy and reliability of the explosion induction period measured. From the point view of the maximum explosion pressure, there was a certain difference between the experimental value and the simulated value, but the overall trend was consistent. As for the maximum pressure, the experimental values were close to the values of the simulated values, and both increased with increasing the aerosol concentration. As for the final pressure value, the simulated value was in good agreement with the experimental value, which reflected the inhibition of the explosion of methane-air mixture by different concentrations of aerosol.

In summary, from the four explosion characteristics of the explosion induction period, the maximum explosion pressure value, the maximum pressure time and the final pressure value, it could be concluded that the simulation value was very consistent with the measured value in the literature [14]. Therefore, the numerical simulation could basically reflect the prevention of the explosion of methane-air mixture by different concentrations of aerosols, and could be treated as a good guide for the study of gas explosion suppression.
5. Conclusions
a. During the suppression process of the methane-air explosion, as the aerosol concentration increased, both the explosion induction period and the time to reach the maximum explosion pressure extended and the maximum explosion pressure slightly decreased. When the aerosol concentration reached a certain threshold, methane-air no longer exploded, which was very consistent with the experimental values.

b. Compared with the experimental values, the data of the explosion induction period, the maximum explosion pressure and the maximum explosion pressure time at different aerosol concentrations obtained by numerical simulation were more accurate, which could provide a good reference for the experimental research.

c. If the ignition occurs first, what happens for the explosion inhibition characteristics of aerosols on methane-air and the effects of the aerosol concentration on pressure and temperature? It needs a further research.

References
[1] Jiang X. S., Du Y., Yan X., et al (2008) On the mechanism and technology for explosion suppression in case of fuel-air mixture in below surface fuel depot. Journal of safety and environment, 8: 134–139.
[2] Lu C., Wang H. B., Zhang Y. P., et al (2019) Experimental on the prevention of gas explosion by nitrogen curtain. Chemical Industry and Engineering Progress, 38(07): 3056-3064.
[3] Chen D. G., Yao Y., Deng Y. J. (2019) The influence of N2/C02 blends on the explosion characteristics of stoichiometric methane–air mixture. Process Safety Progress, 38(2), e12015.
[4] Pei B., Li J., Wang Y., et al (2019) Synergistic inhibition effect on methane/air explosions by N2-twin-fluid water mist containing sodium chloride additive. Fuel, 253: 361-368.
[5] Yu G. M., Liu M. R., Wen X. P., et al (2019) Study on synergistic inhibition of gas explosion by unltrafine water mist-porous material. Journal of China Coal Society, 44(05): 1562-1569.
[6] Dai B., Zhang S. H., Chen Y. H. (2016) Novel cold aerosol fire extinguishing agent performance. Science Technology and Engineering, 16(28): 308-312.
[7] Kibert C. J., Dierdorf D. (1994) Solid particulate aerosol fire suppressants. Fire Technology, 30(4): 387-399.
[8] Liang G. D. (2013) The application of cold aerosol fire extinguishing agent and hot aerosol fire extinguishing agent in the suppression of tunnel fire. Shanxi Science and Technology, 28(4):146-147.
[9] Liu F. Y., Liu T. J., Liu J., et al (2019) Simulation of the motion process of cold aerosol in a narrow tunnel [J]. Fire Science and Technology, 38(01): 124-127.
[10] Zhang X., Ismail M. H. S., Hee C. (2015) Hot aerosol fire extinguishing agents and the associated technologies: a review. Brazilian Journal of Chemical Engineering, 32(3): 707-724.
[11] Xu D. Y., Dai X. Y., Hua M., et al (2012) Numerical simulation of superfine powder extinguishing agent movement released in non-fire room. Journal of Nanjing Tech University (Natural Science Edition), 34(6): 130-135.
[12] Qu L. N. (2010) Experimental research on suppressing gas explosion by K and S-type aerosol. Xi'an: Xi'an University of Science and Technology.
[13] Ren C. X., Sun X., Zhang X., et al (2014) Research on suppressing premixed fuel-air explosion by ultra-fine cold aerosol. Procedia Engineering, 84: 340-346.
[14] Krasnansky M. (2006) Prevention and suppression of explosions in gas-air and dust-air mixtures using powder aerosol-inhibitor. Journal of Loss Prevention in the Process Industries, 19(6): 729-735.
[15] Cao B., Zhang L. J., Zhang C. F., et al (2011) Comparison of FDS and FLUENT applied in the pool fire simulation. Journal of Safety Science and Technology, 7(9): 45-49.
[16] Both A. L., Atanga G., Hisken H. (2019) CFD modelling of gas explosions: Optimising sub-grid model parameters. Journal of Loss Prevention in the Process Industries, 60: 159-173.
[17] Crowe C. T., Troutt T. R., Chung J. N. (1996) Numerical models for two-phase turbulent flows. Annual Review of Fluid Mechanics, 28(1): 11-43.

[18] Zhou L. X., Chen T. (2001) Simulation of swirling gas–particle flows using USM and k-ε-kp two-phase turbulence models. Powder Technology, 114(1-3): 1-11.

[19] Rahul G. (2009) Modeling and simulation of two-phases flow. Ames: Iowa State University.

[20] Yan C. J., Fan W. (2005) Combustion. Northwestern Polytechnical University Press, Xi’an.