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Numerical Simulation on Flame Propagation Characteristics of Coal Dust Explosion in Diagonal Structure Network

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In order to study the propagation characteristics of coal dust explosion in the angular branch, gambit software is used to establish a model of the pipe network and to divide the grid. Based on the process of coal dust explosion, several theoretical models for the propagation characteristics of coal dust in numerical simulation are expounded. Using FLUENT to simulate a coal dust explosion in the corner branch, the characteristics of flame temperature and air flow velocity propagation and the pressure propagation characteristics in the angular branch are analyzed. Then, the propagation characteristics of flame temperature are studied. The results show that the length of the coal dust explosion flame area is far greater than the incidence of coal dust and the length of the ignition zone, and is influenced by the branch direction of the pipe network and the bifurcation point, and the flame propagating outward from the explosion source is asymmetric. The propagation of the blast flow basically corresponds to the flame propagation, and the two are accompanied by the flame.

1. Introduction

Coal dust explosion accidents in the diagonal structure network are extremely serious (Bi, 2017), in China's coal mine history, there have been many serious coal dust explosions in the diagonal structure network. The destruction extent of a coal dust explosion depends on the flame propagation and the development and variation characteristics of explosion waves during the explosion process (Yu et al., 1995; Fei, 1997; Zhou, 2001). Therefore, it is of great necessity to study the flame propagation law of coal dust explosions. Traditional research is based on experimental methods. Duan et al., (2012) have studied the flame propagation law of coal dust explosions in a straight line through experiments; the results showed that maximum flame velocity and propagation distance are not proportional to the coal dust, but the maximum flame velocity is reached at a certain mass concentration. Cao et al., (2014) calculated the empirical formula of flame propagation speed and temperature under specific conditions through a large number of experimental data. Li Yucheng and Si (2018) obtained the influence factors of the flame propagation characteristics of coal dust explosions and arrived at predictions of flame propagation. However, with the development of computational fluid mechanics and computer hardware technology, the numerical simulation method has become an important means to study the process of dust explosion in the network space. The method is very economical and rapid, and the results can show the velocity field, temperature field, and particle trajectory of different times in the calculation area. Rongjun Si and others developed the numerical simulation system of gas and coal dust explosions with the help of the commonly used flow field simulation platform. Meanwhile, Licong Zhang and others used numerical simulation to study the effect of obstacles on methane and coal dust explosion propagation. Runzhi Li built a two-dimensional numerical model with the help of the FLUENT platform, and simulated the process of coal dust explosions. Researchers both here and abroad have comprehensively studied the explosion of gas dust by numerical simulation, but there is little research on dust explosion in the diagonal structure network. In this paper, numerical simulation research on the self-designed coal dust explosion diagonal structure network device is carried out. Thus, the scope of coal dust explosion accidents is obtained, and the

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function of early assessment is realized. This provides theoretical guidance for the installation of explosion protection facilities.

2. Geometric model establishment and grid division of diagonal structure network

Use GAMBIT to draw a three-dimensional geometric model of a diagonal pipe and divide the grid (Figure 1.1). The total length of the model is about 32m, the diagonal branch is about 10m, and the diameter is 0.5m. First, the quadrilateral/triangular mixed surface mesh is divided by pave (unstructured grid), and the whole geometry is divided into Tet/Hybrid (Tetrahedron/ mixture) grid with TGrid, and the total number of body grids is 520789.

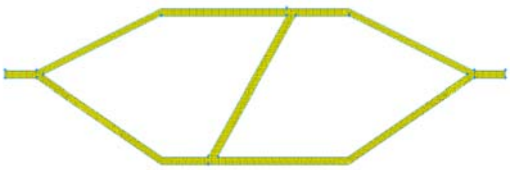

Figure 1: Geometric model diagram

3. Theoretical model of coal dust explosion propagation characteristics

From the process of coal dust explosion, It can be seen that the main models involved in the dust explosion include the basic conservation model, the coal dust particle turbulent combustion model, the gas phase turbulent combustion model, the gas phase turbulence model, the gas-solid two-phase flow model, and the radiation heat transfer model. In order to simplify the model description, the coal dust is regarded as a discrete phase, and only the radiation heat transfer between the coal dust and the continuous phase and the coal dust particles is considered, and the friction collision between the particles is not considered.

3.1 Gas phase turbulence model

In this paper, we use the double equation model in the Reynolds Averaged Numerical Simulation (RANS) − the standard K-ε model. The model is a commonly used turbulence model with industrial application. It is relatively simple and easy to use. The convergence and accuracy of the model are highly consistent with the requirements of engineering calculations. But the ε equation, which cannot be calculated on the wall, is only suitable for the simulation of the flow field in full turbulence and cannot be used for the laminar flow of a low Reynolds number. Therefore, the wall function must be used as the near-wall treatment. The wall functions proposed by Lauder and Spalding are used to deal with the turbulent flow near the wall. In the mean velocity region, the wall function equation is:

$$U^* = \frac{1}{k}\ln(Ey^*),\ y^* = \frac{\rho C_\mu^{1/4} k_p^{1/2} p'}{\mu}$$

3.2 Gas phase turbulent combustion model

The turbulent combustion of gas in coal dust explosions is mainly the combustion of volatile gas released from coal dust particles after heating, The combustion is fast and violent, so the eddy dissipation (Eddy-Dissipation) model, which is one of the limit reaction rate models, is used.
Considering the interaction between the chemical reaction and turbulent mixing, the model can simulate most of the fast and violent gas-phase combustion processes. In order to simplify the calculation, the reaction mechanism of the two steps is as follows:

h_v-vol+ O_2 CO + CO_2+H_2O +N_2 (1)

O_2+2CO =2 CO_2 (2)

The overall reaction rate is coupled to the flow field. The rate of combustion depends not only on the chemical kinetic field, but also on the flow field. In the reaction r of volatile gases' turbulent combustion, the formation rate $R_{i,r}$ of matter i is:

$$R_{i,r} = v_{i,y} \bullet M_{w,i} \bullet A \bullet \rho \bullet \frac{\varepsilon}{k} \bullet \min\left(\frac{Y_R}{v_{R,r} \bullet M_{w,R}}\right) \tag{3}$$

In the formula: Y_R is the mass fraction of the reactant component; A is the rate constant of reaction (1), and takes A=4.0, $M_{w,I}$ is the gas molar mass.

The formation rate of CO_2 in the oxidation process is R:

$$R = v \bullet M_w \bullet B \bullet \rho \bullet \frac{\varepsilon}{k} \bullet \left(\frac{\sum_p Y_p}{\sum_j^N v_j^n \bullet M_{w,j}} \right) \quad (4)$$

In the formula: Y_P is the mass fraction of the composition of the product; B is the rate constant of reaction (2), and is taken as B=0.5.

3.3 Coke combustion model

The extended diffusion dynamic control combustion model is used. The combustion rate of coke is controlled by two factors: the rate of oxygen diffusion to the surface of the coke and the kinetic rate of chemical reaction. The diffusion rate constant of oxide and oxidant to the particle surface is D_0:

$$D_0 = C_1 \frac{\left[\left(T_p + T_g\right)/2\right]^{0.75}}{d_p} \quad (5)$$

In the formula: Tp is the particle phase temperature, K; Tg is the gas-phase temperature, K; dp is the average diameter of the particles, M. The kinetic reaction rate constant of the coke combustion model is:

$$\Re = C_2 e^{-\left(\varepsilon/RT_y\right)} \quad (6)$$

Combining the diffusion rate constant D_0 and the kinetic reaction rate constant, a weighted calculation is carried out. The calculation expression of the coke burning rate is obtained:

$$\frac{dm_p}{d_t} = -\pi \bullet d_p^2 \bullet P_{ox} \bullet \frac{D_0 \bullet \Re}{D_0 + \Re} \quad (7)$$

In the formula: The dm_p/d_t is the mass change rate of residual carbon particles, kg/s; Pox is the Pa of the gas-phase oxidant around the particles.

3.4 Other models

The radiation heat transfer effect is considered and the P1 radiation model is adopted.
The particle discrete phase flows into the gas phase by the Euler-Lagrange method. The particles are regarded as discrete phases, and the gas is regarded as a continuous phase. The particle trajectory model is based on the particle random orbit model, which has a short computation time and small workload. It is more suitable for simulating the reaction of volatile coal dust.

4. Numerical simulation and result analysis of coal dust explosion in diagonal branch

4.1 Boundary condition, initial condition and flow field

Boundary conditions of passages and walls as in Tables 1, 2:

Table 1: Boundary condition of entrance and exit

Boundary	Relative pressure /Pa	Turbulence intensity /%	Hydraulic diameter /m	temperature /k	O_2 mass fraction%
entrance	50	10	0.25	300	23
exit	0	10	0.25	300	23

Table 2: Boundary condition of walls

Boundary condition	Material	Tube wall density / kg·m-3	specific heat / J·(kg·K)-1	Thermal conductivity / W·(m·K) -1	Internal scattering rate	temperature / k
walls	steel	8030	502	16.27	0.5	300

Different wall roughness coefficients are given to each branch of the tube network. In order to, the air flow passes through the diagonal branches after being initialized in the flow field and cold reaction, and meets the wind speed limitation of the roadway.

Because the working face is located in the diagonal branch, the coal dust source is uncertain and the fire source is caused by an external cause. This simulation randomly selects the location of the discrete phase coal dust particles – the middle and lower parts of the diagonal branch, and the incident conditions are shown in Table 3.

The initial velocity assignment is based on the following: Coal sample tube parameters of the small-size straight-line pipe coal dust explosion test are 0.02 M inside diameter, 0.2m of coal sample tube length, 0.95 of inner wall roughness of the coal sample tube, 5 x 10^4 Pa of initial dust pressure, 1.29 kg/m^3 air density, and 9.8 m/s^2 gravity acceleration. First, it is calculated that the pressure gradient in the coal sample tube is $(5\times10^4)/(1.29\times9.8\times0.2)=19379.84$. Then it is calculated that the specific resistance of the coal sample pipe is $(10.3\times0.95^2)/(0.02^{5.33})\approx10^{10}$. Finally, the volume flow of high-pressure air flowing through the coal sample tube is calculated to be $(19379.84/10^{10})^{1/2}=0.001354$ m^3/s. According to the cross section area of the coal sample tube, the air velocity of the coal sample tube outlet is calculated to be $0.001354/(\pi\times0.01^2)=4.31$ m/s. Considering the friction between the air flow and coal dust particles, the initial incident velocity of particles is slightly less than that of the coal tube outlet, so 4m/s is taken. Quality flow assignment basis: When the dusting powder time is 0.2S, the coal sample will move 0.8m from the exit movement in 0.2S. in the simulation. The concentration of coal dust explosion is 300 g/m^3 (the strongest explosive power is 300~500g/m^3), and the mass flow rate is$300\times0.8\times0.5^2/0.2=0.3$ kg·s^{-1}.

Initial high temperature ignition zone: The Patch function is used to define the high-temperature ignition zone of the cylinder above the dust injection zone in the diagonal branch, which is equivalent to delineating a 0.2m-long cylinder high-temperature zone in the tube. The temperature in the high temperature zone is 1500 K (a straight-line pipe experimental study shows that the minimum ignition temperature of a lignite coal dust cloud is 963K and 1500K meets the minimum ignition temperature requirement)..It is used to trigger the chemical reaction of a coal dust explosion. In a high-temperature zone, the mass fraction of O_2 is 23%, the mass fraction of H_2O is 0.01%, and the mass fraction of CO_2 is 0.01%.

Table 3: Initial incident condition of coal dust particles in discrete phase

Material	diameter/μm	type	initial temperature/k	Incidence direction and velocity/m·s-1	mass flow/kg·s-1	time/s
Coal-hv	75	Group injection	300	x=4, y=4	0.3	0.2

The physical properties of the combustion particles are as follows in Table 4:

Table 4: Physical properties of combustion particles

density / kg·m-3	Cp / J·(kg·K)-1	Volatile / %	Vaporization temperature / k	Binary diffusivity / m2·s-1	Swelling coefficient	Burnout stoichiometric ratio	Combustible fraction / %	Heat of reaction for burnout / J·kg-1
1000	1100	36.88	773	3×10-5	2	2.67	36.7	3.29×107

The heat absorbed by the solid wall is 2% of the heat released from coke burning. After initializing the flow field and calculating the convergence, the direction of the overall air flow is from left to right, the direction of the wind propagation in the diagonal branches is down-up, and the air volume of each node is balanced.

4.2 Simulation results and analysis of coal dust explosion

4.2.1 Analysis of flame temperature propagation characteristics in Z=0.25 section

According to the above settings, the explosion process in the diagonal branches is simulated by FLUENT software, and the flame temperature cloud images at different times are obtained, as shown in Figure 2. The red, high-temperature region represents the flame, and the other high-temperature regions are mainly caused by the diffusion and propagation of the flame temperature.

(1) When the coal dust is ignited in 0.02s, the flame is centered around the explosion source, and propagates rapidly up and down in two directions. At 0.05s, the flame forward reaches the upper and lower bifurcations, and the temperature of the flame front is the highest, reaching 2800K. At 0.05s, the flame front reaches the upper and lower bifurcations, and the flame front surface temperature is the highest, reaching 2800K. After the flame front, due to the decrease of oxygen concentration and volatiles, the flame attenuates and extinguishes, and there is no obvious change rule in the attenuation process. From the above flame propagation process, it is found that the flame propagation length is much larger than the coal dust incident and ignition zone length, and the flame almost spreads throughout the pipeline. This result can be explained by the mechanism of coal

dust explosion propagation: Coal dust forms coal dust clouds in a cavity; at first, some dust particles are burned after being ignited and the heat released is transmitted to the surrounding coal dust and burned, so that the flame starts to spread outward quickly. At the same time, because of the constraint effect caused by the small radius of the physical model, the flame wave spreads rapidly to the wall of the tube, which induces turbulence, wrinkles the flame, and accelerates the flame surface. A large amount of heat is released from the combustion, and a large number of gases are rapidly inflated. The action of the preflamed pressure wave forces some unburned mixtures to move along with the flame area, and they are ignited at the same time. This positive feedback effect accelerates the combustion and causes the length of the flame region to be far greater than the length of the ignition zone.

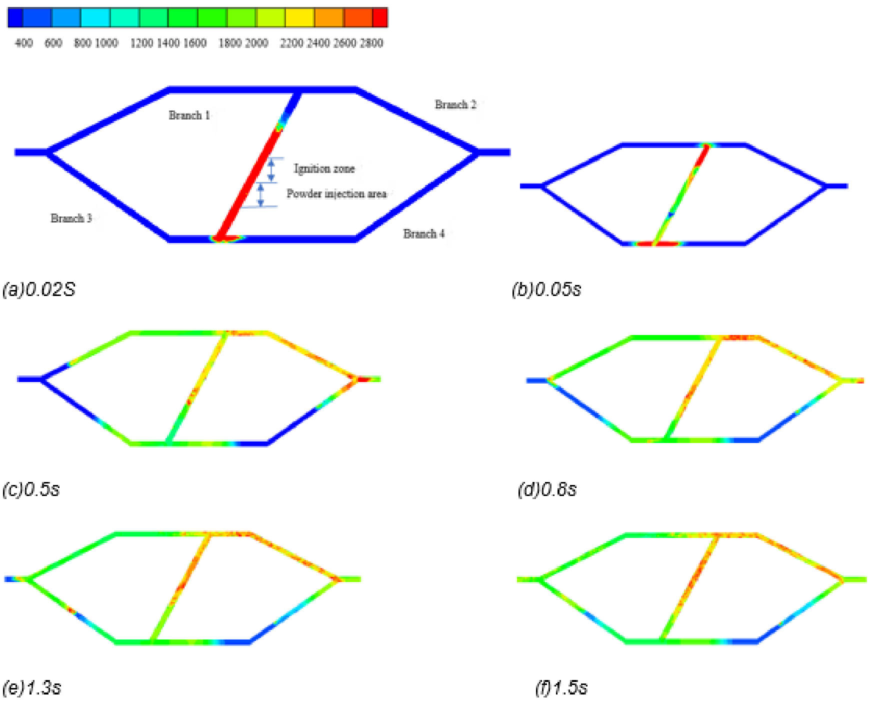

Figure 2: Flame temperature cloud at sections of Z=0.25 at different times

At the same time, from the analysis of the flame propagation process nephogram, the flame propagates rapidly from the explosion source to the upper and lower directions in an asymmetrical state, and on the left and right bifurcations, they are first propagated in the direction of reentry, that is, branches 3 and 4.Then it is in the exit and entrance branch of the horizontal direction, and the temperature of the flame at the bifurcation point is higher than that of each point before and after. It shows that the greater the turbulence is, the more favorable the flame propagation. Because of the special structure of the network, a change of the asymmetric sections and the bifurcations of the flame is encountered during the propagation process, where the turbulence intensifies and the combustion reaction is accelerated. This is also different from the transmission of straight lines.
(2) The flame propagation velocity first increases and then decreases, and there is a critical value which is caused by deflagration to detonation. The turbulence caused by the shock wave will also cause a subsequent accelerated propagation of the flame and a longer distance of flame propagation.

4.2.2 Analysis of air velocity propagation characteristics of Z=0.25 cross section

(1) After the explosion of coal dust, a large number of explosive products are generated. The explosion temperature makes the explosion products expand rapidly and causes them to be in a high-speed state and produce impact air flow. At the initial stage of the explosion, the velocity of air flow is relatively small, with the maximum value of 0.02s being only 44m/s, then the velocity of the air flow increases sharply, and the maximum air flow velocity of 0.05s reaches 499m/s, which is the transition of deflagration to detonation. After that, the air flow velocity rapidly attenuates due to friction loss. Due to the hindrance at the bifurcation and turning points, a wind flow is stimulated, which leads to increased wind velocity; that is, the velocity of the air flow in the fork and the turn increases and then decreases. Compared with the flame temperature cloud, the propagation process of the impacting air flow basically corresponds to the flame propagation, which shows

that they accompany each other, The high-speed propagation of the impinging air increases the propagation range of the high-temperature flame, while the heat of the flame expands the air flow and accelerates its propagation.
(2) Monitoring data show that when 1.1s, part of branch 4 had a minimum air flow velocity, namely 0.3m/s. This is because the flame forward propagating to the right side of branch 4 from the lower part fork in the diagonal branch and the flame transmitted to branch 4 by the two branches passing through the bifurcation will all attract the front oxygen to burn. This is equivalent to pulling the air in the middle, resulting in a minimum velocity of about 0.3m/s.

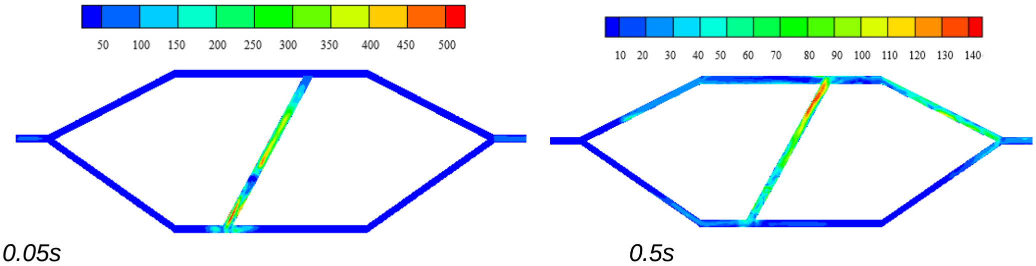

Figure 3: Air velocity clouds at section of Z=0.25 at different times

5. Conclusion

(1) After the ignition and explosion, the diagonal branch of the length of the flame zone is much larger than that of the coal dust and the ignition zone, which almost propagate the entire pipeline. Compared with the large tunnel experiment, due to the constraint effect produced by the small radius of the physical model and the special structure of the pipe network, the flame forms turbulence when it collides with the tube wall, which aggravates the combustion reaction. At the same time, there is an expansion of a large number of gases after burned and unburned volatiles are propagated along the pipeline, and the flame propagation is accelerated. The flame propagating rapidly from the explosion source to the upper and lower directions is asymmetrical, which is a notable feature of flame propagation of coal dust explosions in the diagonal branch.
(2) The propagation of the impacting air flow basically corresponds to the flame propagation, which shows that they are associated. The high-speed propagation of the impacting air increases the propagation range of the high-temperature flame. At the same time, the heat of the flame expands the air flow and accelerates its propagation.
(3) The numerical simulation results are basically consistent with the theoretical results. However, the maximum flame temperature value is higher than the theoretical and experimental temperature values, which is related to the simplified assumptions of the selected models and the setting of some empirical constants .Further research is needed.

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Reference

Bi M.S., 2017, Gas and dust explosion prevention engineering, first edition. Beijing: Chemical Industry Press, 1-3.
Cao W.G., Xu S., Liang J.Y., 2014, The propagation characteristics of flame in the process of pulverized coal dust explosion, Explosion and Impact, 34(5), 586-593, DOI: 10.11883/1001-1455(2014)05-0586-08
Duan Z.W., Li Z.Q, Jing G.X., 2012, Experimental study on flame propagation law of coal dust explosion in straight line, Chinese Journal of safety science, 22(3), 103-108.
Fei G.Y., 1997, Experiment of coal dust explosion caused by gas explosion in single entry roadway, Coal Engineers, (4), 16-19.
Si R.J., 2018, Numerical simulation study on propagation of mine gas and coal dust explosion, Chinese Journal of Safety Science,18(10), 82-86, DOI: 10.16265/j.cnki.issn1003-3033.2008.10.013.
Yu D.M., Feng C.G., Zeng Q.X., Guo X.Y., 1995, The damage explosions and the division of their injury regions, China Safety Science Journal, 5(S), 13-17, DOI: 10.16265/j.cnki.issn1003-3033.1995.s2.004.
Zhou T.Q., 2001, Explosion dynamics and applications, First edition. Hefei: University of Science and Technology of China press, 93-94.