Large Eddy Simulation of Premixed CH\(_4\)/Air Deflagration in a Duct with Obstacles at Different Heights

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**ABSTRACT:** In this work, the propagation of CH\(_4\)/air deflagration flames in three semi-confined ducts with different obstacles was numerically investigated using large eddy simulation (LES). The shape of the premixed flame, flow field structure, and overpressure characteristics of the interaction between the flame and the obstacle are simulated accurately in three ducts with obstacles of different heights. The results show that the structure of the flame is changed by the presence of obstacles, and a change in the shape of the hemispherical conical brush appears, and a flame vortex is generated by the entrapment of unburned premixed gas on the left side of the obstacles. In the process of CH\(_4\)/air deflagration, the existence of obstacles would lead to the change in combustion velocity and overpressure relief velocity and then have a certain influence on the peak of overpressure and the shape of the premixed flame.

1. INTRODUCTION

In recent years, with the development of industries, more and more combustible gas are utilized in our industrial production, resulting in explosion accidents in a variety of industrial places, especially methane/air in the closed area of deflagration, likely causing irreversible losses to personnel, equipment, and production processes. Especially, when the combustible gas explosion occurs when there are all kinds of obstacles of space, gas combustion will encounter all sorts of obstacles and unpredictable situations, such as the obstacles under the action of all kinds of vortex formation, flame surface folds, flame area increases so that the flame propagation speed is faster, and burning fuel causing a greater loss.\(^1\) In addition, methane is the main component of natural gas and is generally recognized as a clean fuel in industry,\(^5\) the study of the interaction of methane/air with pipe walls and obstacles in pipelines has also become a hot topic.

The dynamics of premixed combustion in pipelines is an important subject in combustion science. Due to the wall conditions and even under certain conditions, premixed flames develop into detonation. Especially, flames interact with the pipe wall and obstacles, and the flame propagation speed and the pressure on the surrounding environment will be significantly increased.\(^9\)\(^−\)\(^11\) Therefore, the research of the flame and pipe wall and obstacle interaction mechanism and the resulting combustion mechanism and changes in the flow field structure to effectively prevent the occurrence of the gas explosion accident and reduce disaster loss has great significance.\(^12\)\(^−\)\(^15\) When the premixed flame interacts with such obstacles in the process of propagation, the shape of the flame, the propagation velocity of the flame, the structure of the flow field, and the explosion overpressure will change significantly compared with the space without obstacles. Therefore, scholars around the world have carried out in-depth research on the explosion mechanism, the characteristics of propagation, and influencing factors of gas explosion under the conditions of barriers.\(^16\)\(^−\)\(^18\)

In the past few years, a great deal of research has been done in the field of large eddy simulation (LES) of turbulent combustion, but many fundamental problems need to be solved to fully realize the predictive potential of combustion LES. Pitsch\(^4\) focused on the fundamental differences between Reynolds-averaged Navier–Stokes and LES combustion models for non-premixed and premixed turbulent combus-
tions. Wen \textit{et al.}\(^6\) conducted LES of Darmstadt turbulent methane/hydrogen flames to study two different flames and two different techniques used to access the flamelet libraries. By analyzing the differential diffusion parameters, the reasons for the different performances of the small flame models were discussed. Wen \textit{et al.}\(^15\) also studied three different methane/
hydrogen flames. The effects of differential diffusion, stretching, and layering on the applicability of the small flame model are studied in detail. Fiorina et al.\textsuperscript{16} compared five different low-Mach LESs with the experimental turbulent stratified flame. Qualitative comparisons of instantaneous snapshots of the flame show differences in the size of the resolved flame wrinkling patterns, which resulted from the effect of the LES combustion model on the flame dynamics and the different simulation strategies in terms of grids. Oh et al.\textsuperscript{16} studied the explosion characteristics of gas in pipelines with built-in obstacles by changing the shape, size, and gas concentration of obstacles. Wang et al.\textsuperscript{19} studied the characteristics of ethylene deflagration to detonation in the pipeline by changing the width of the pipeline through calculation. Di Sarli et al.\textsuperscript{20} used particle image velocimetry to capture the vortex structure behind the obstacle and pointed out that the interaction between the flame and the vortex is the main reason for the acceleration of the flame and the change in the flame shape. Xu et al.\textsuperscript{18} conducted LES with a method combining TFC (turbulent flame closure) subgrid combustion model proposed by Zimont and Battaglia\textsuperscript{21} to simulate the deflagration propagation process of methane/air premixed in a pipeline containing three flat obstacles and found that the subgrid combustion model could accurately predict the main characteristics of the flame structure, overpressure, and flame propagation velocity. Di Sarli et al.\textsuperscript{20} analyzed the influence of the number of obstacles on the propagation characteristics of premixed flame through experiments and found that the explosion overpressure would increase with the increased number of obstacles, but there was a certain upper limit for the increase in overpressure. After reaching the upper limit, the overpressure curve would decrease with the increase in the number of obstacles. Mastri et al.\textsuperscript{22} studied the characteristics of the premixed flame in obstacles of different shapes by changing the blocking ratio, and the results showed that compared with triangular obstacles and round obstacles, square obstacles had the greatest influence on the flame propagation process. Fairweather et al.\textsuperscript{23} pointed out that the propagation of the methane/air premixed flame in the barrier pipe is a process of a laminar flame changing to a turbulent flame. Wen et al.\textsuperscript{24} conducted a comparative test on parallel and staggered obstacles in combination with the number of obstacles and their positions in the pipeline and found that under the structure of staggered obstacles, the peak overpressure and flame velocity of deflagration were relatively high. Mastri et al.\textsuperscript{22} experimentally analyzed the influence of the number of obstacles on the propagation characteristics of the turbulent premixed flame and found that the explosion overpressure increased with the increase in the number of obstacles, but there was an upper limit, and when the upper limit was exceeded, the explosion overpressure decreased with the increase in the number of obstacles. Some scholars studied the explosion characteristics of oil and gas in a narrow and long confined space with two side branches on the basis of LES and pointed out the reason why the interaction between the flame and flow field in the pipeline led to the flow field turning to turbulence and the deformation of flame front folds. Some experimental studies\textsuperscript{11,22,25–27} have been partially successful in understanding this complex mechanism of obstacle induction; however, the exact mechanisms of the flame structure, velocity, and resulting overpressure are not well understood by experimental measurements alone. Also, what kind of obstacles would cause changes in flame speed, shape, and overpressure to better prevent the damage caused by the explosion? In this work, the effect of obstacles on methane/air flame propagation in semi-open ducts was studied. In LES, the power law flame ruffle model proposed by Charlette et al.\textsuperscript{28} was used to capture the dynamics of flame propagation, and three obstruction channels of different heights were considered to explore the effects of the methane/air flame structure, propagation velocity, and overpressure comparison.

LES can capture the shape of the flame, the velocity of the flame front, and the structure of the flow field, indicating that LES is suitable for studying the propagation characteristics of the premixed flame in the obstructed pipeline. Meanwhile, by changing the height of the obstacles, the influence on the promotion or inhibition degree of premixed flame propagation under different conditions is investigated. It is helpful to predict the flame propagation characteristics of premixed methane/air in barrier piping to prevent gas explosion accidents and reduce disaster losses.

2. LES MODEL

The continuity equation, momentum conservation equation, and energy conservation equation of LES are filtered by the original N–S (Navier–Stokes) equation. In the simulation of gas deflagration in tubes, the compressibility of the mixture must be considered, and this filtering is usually Favre filtering. These filtered equations in LES can be referred to in refs \textsuperscript{29} and \textsuperscript{30}. The subgrid turbulent stress tensor in the momentum equation needs to be given by the subgrid eddy viscosity model. The dynamic Smagorinsky–Lilly eddy viscosity model\textsuperscript{31} is used in this work, and the subgrid turbulent heat flux in the energy equation is calculated according to the gradient hypothesis. The filtered continuity equation and momentum equations are, respectively

\[
\frac{\partial \rho \overline{U}_i}{\partial t} + \frac{\partial (\rho \overline{U}_i \overline{U}_j)}{\partial x_j} = -\frac{\partial \rho \overline{U}_i}{\partial x_j} \left[ \frac{\partial Y_i}{\partial t} - \rho U_j \overline{U}_i \right]
\]

(2)

In this work, the conservation equation of the species is solved using the reaction process variable \(c\). The progress variable is defined as a normalized sum of the product species mass fractions \(c = Y_c/Y_{c,eq}\) where \(Y_c\) is the product mass fraction and superscript \(eq\) denotes chemical equilibrium. If the progress quantity is solved, the concentration of each species can therefore be solved directly. Using the reaction process variable \(c\) means that the complex structure inside the flame has been simplified to only one variable. The original conservation equation of the reaction process variable is

\[
\frac{\partial c}{\partial t} + \nabla \cdot (\rho c \mathbf{U}) = \nabla \cdot (\rho D \nabla c) + \omega_c
\]

(3)

The first term on the left side of this equation is the unsteady term, and the second term is the convection term. The first term on the right side of the equation is the diffusion term of the species, and the second term is the reaction source term. All of the species concentrations here are actually replaced by the reaction process variable \(c\). The conservation equation of the reaction process variable after Favre filtering is
\[
\frac{\partial \bar{\rho} \bar{c}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{u} \bar{c}) + \nabla \cdot (\bar{\rho} (\bar{u} c - \bar{u} \bar{c})) = \nabla \cdot (\rho D \nabla \bar{c}) + \dot{\omega} \bar{c} \tag{4}
\]

In this equation, there are three terms that cannot be closed using other equations in the conservation equations. The first term is the third term on the left side of the equation. \(\nabla \cdot (\bar{\rho} (\bar{u} c - \bar{u} \bar{c}))\) is called the subgrid flux of the reaction progress variable. This term is called the subgrid flux of the reaction progress variable. Similar to the solution method of the subgrid convection term of the heat equation, this term is also calculated by the gradient hypothesis.\(^{32}\) The other terms are the two terms at the right end of the abovementioned equation. The closed problem of these two terms is the so-called subgrid combustion model problem.

According to flame surface theory,\(^{33}\) these two items can be expressed as
\[
\bar{\rho} \omega \nabla \bar{c} = \nabla \cdot (\rho D \nabla \bar{c}) + \dot{\omega} \bar{c} = (\rho \omega) \sum \bar{S} \Xi \nabla \bar{c} \tag{5}
\]

where \(\sum\) is the surface density of the flame, which is defined as the area of the flame surface per unit volume, \(\bar{w}\) is the displacement speed of the flame surface, and \((\rho \omega)\) represents the average displacement speed on the flame surface. \((\rho \omega)\), \(\sum\) can be approximated as the product of the density of the fresh gas and the laminar flame speed. The flame surface density can be expressed as the product of the reaction progress variable gradient and a correction factor by introducing a wrinkle factor.\(^{32}\) With the abovementioned approach, eq 6 can be further transformed into
\[
\bar{\rho} \omega \nabla \bar{c} = (\rho \omega) \sum = \rho \bar{S} \Xi \nabla \bar{c} \tag{6}
\]

The expression of the wrinkle factor is the subgrid turbulent combustion model used in our simulation. This wrinkle factor can simultaneously close the filtering diffusion term and filtering reaction source term in the reaction progress variable equation. The energy equation based on the solution of the progress quantity is
\[
\frac{\partial \bar{h}}{\partial t} + \nabla \cdot (\bar{h} \bar{u}) = \nabla \cdot \left( \frac{k + l}{c} \nabla \bar{h} \right) + \rho \omega \nabla \bar{c} H_{comb} V_{fuel} \tag{7}
\]

where \(k\) and \(l\) are thermal conductivity and turbulent thermal conductivity, respectively, \(H_{comb}\) is the heat of combustion for burning 1 kg of fuel, and \(V_{fuel}\) is the fuel mass fraction of the unburnt mixture.

The formula of the wrinkle factor in the simulation in this work uses a power law expression proposed by Charlette et al. as\(^{28}\)
\[
\Xi = \left( 1 + \frac{\Delta}{\eta_\Delta} \right)^\beta = \left( 1 + \frac{\Delta}{\eta_\Delta} \right)^\beta = \left( 1 + \min \left\{ \frac{\Delta}{\eta_\Delta}, \Gamma \left( \frac{\Delta}{\eta_\Delta}, \frac{\bar{u}}{S_L}, \text{Re}_\Delta \right) \left( \frac{\bar{u}}{S_L} \right) \right\} \right)^\beta \tag{8}
\]

In this formula, the wrinkle factor is expressed as a function of the grid scale, the inner cutoff scale, and the exponential \(\beta\). The inner cutoff scale needs to be calculated using an efficiency function. Based on the results of a DNS (direct numerical simulation), Colin et al.\(^{34}\) expressed the efficiency function as a correlation between the subgrid scale and the laminar flame thickness ratio, the subgrid turbulent velocity and the laminar flame speed ratio, and the subgrid Reynolds number. In the model proposed by Charlette et al.,\(^{28}\) which is also the model used in this work, the efficiency function can be expressed as
\[
\Gamma \left( \frac{\Delta}{\eta_\Delta}, \frac{\bar{u}}{S_L}, \text{Re}_\Delta \right) = \left( \frac{f_u a + f_\Delta a}{a} \right) \eta^{2} + f_\text{Re}^{2} a \tag{9}
\]

where
\[
f_u = 4 \left( \frac{27C_k}{110} \right)^{1/2} \left( \frac{18C_k}{55} \right) \left( \frac{U_o}{S_L} \right)^2 \tag{10}
\]
\[
f_\Delta = \left[ \frac{27C_k}{110} \left( \frac{\Delta}{\eta_\Delta} \right)^{4/3} - 1 \right]^{1/2} \tag{11}
\]
\[
f_\text{Re} = \left[ \frac{9}{55} \exp \left( - \frac{3}{2} C_k a^{4/3} \Xi \right) \right]^{1/2} \tag{12}
\]
\[ a = 0.6 + 0.2 \exp \left( -0.1 \frac{u'_{\Delta}}{S_{L}} \right) - 0.2 \exp \left( -0.01 \frac{\Delta}{\delta_i} \right) \]  
\( C_k = 1.5, \quad b = 1.4 \)  
\[ u'_{\Delta} = \frac{\rho L_s |\delta|}{\rho L_s} = L_s |\delta| = C_s \Delta |\delta| \]  
\[ \frac{S_1 \delta}{D} = \frac{S_1 \delta}{\nu} = 4 \]  
\[ \text{Re}_{\Delta} = \frac{u'_{\Delta} \Delta}{\nu} = 4 \frac{u'_{\Delta}}{\delta_i S_{L}} \]  

The exponent \( \beta \) in the power expression is 0.5 as recommended. According to the relation between the subgrid turbulent velocity and the eddy viscosity and the correlation between the integral scale and the subgrid scale, the subgrid turbulent velocity can be expressed as \( 32 \)

\[ u'_{\Delta} = \frac{\rho L_s |\delta|}{\rho L_s} = L_s |\delta| = C_s \Delta |\delta| \]  

It should be noted that \( C_s \) in eq 15 is a dynamic value in the dynamic Smagorinsky–Lilly model. In addition, based on the approximate dimensionality of the laminar flame scale \( 35 \)

\[ \frac{S_1 \delta}{D} = \frac{S_1 \delta}{\nu} = 4 \]  

The Reynolds number at the subgrid scale can therefore be expressed as

\[ \text{Re}_{\Delta} = \frac{u'_{\Delta} \Delta}{\nu} = 4 \frac{u'_{\Delta}}{\delta_i S_{L}} \]  

### 3. NUMERICAL DETAILS

The simulated geometric structure is shown in Figure 1a with a size of 100 mm \( \times \) 100 mm \( \times \) 408 mm. There are six layers of symmetrical obstacles in the pipeline. The size of the obstacles arranged symmetrically is showed in Table 1. In order to study the influence of the stepped obstacle on the deflagration flame propagation in the pipe, in addition to the mentioned obstacle structure, two groups of obstacles, gradually lower and gradually higher, are also set up in the work, as shown in Figure 1b,c.

The pipe is initially filled with a methane/air mixture with an equivalence ratio of 1. The left end of the pipe is closed, and the right end is open. The adiabatic boundary conditions and no slip boundary conditions are applied to the entire outer wall. The outlet of the pipe is set to a pressure outlet, which means that the pressure at the outlet is set to equal atmospheric pressure. A structured hexahedral grid was used with a uniform grid size of 1 mm. This grid size has been demonstrated in studies to be sufficient to capture the vast majority of turbulent–flame interaction structures in small-scale obstructed pipes. \( 30-38 \) This is enough to satisfy the criterion raised by Pope. \( 29,47 \) It was found that \( \Xi \) is relatively insensitive to turbulence levels and varies from unity to less than 1.3 over a wide range of mesh sizes.

At the initial moment, the temperature of the whole simulation region is set to 300 K, and the reaction progress variable is set to 0. This setting indicates that the whole simulation region is in the unburned state. The ignition strategy in the simulation is set to a hemispherical region with a radius of 5 mm at the left end, and the parameters of the hemispherical region were set as the parameters of the equilibrium state. The setting of equilibrium-state parameters in the hemispherical region mainly includes two parts. One is the reaction progress variable \( c \) set as 1, indicating that it is in the state of complete combustion, and the other is the adiabatic flame temperature when the equivalence ratio of the methane/air mixture is 1, namely, 2258 K. The surface of the flame formed by the ignition is refined to ensure that the early flame is smooth enough.

The finite-volume method is used to discretize the equations involved in LES of the deflagration flame. The diffused terms in all equations were discretized using a second-order central difference scheme, while the convective terms were discretized using a bounded central difference scheme. The unsteady term is discretized using a second-order implicit scheme. The time step is \( 5 \times 10^{-6} \) s, and this time step ensures that the Courant

### Table 1. Schematic Diagram of the Obstacles

| \( H \) | obstacle 1 (mm) | obstacle 2 (mm) | obstacle 3 (mm) | obstacle 4 (mm) | obstacle 5 (mm) | obstacle 6 (mm) |
|---|---|---|---|---|---|---|
| equal | 38 | 38 | 38 | 38 | 38 | 38 |
| lower | 38 | 33 | 28 | 23 | 18 | 13 |
| higher | 13 | 18 | 23 | 28 | 33 | 38 |

![Figure 2](https://doi.org/10.1021/acsomega.1c03814) 
Figure 2. Field profiles of the three-dimensional structure on the iso-surface \( \varepsilon = 0.9 \) at different propagation stages, when the obstacle sets are (a) equal, (b) lower, and (c) higher.
number is less than 1 throughout the calculation. The commercial software tool Fluent 18.2 was used to implement the abovementioned simulation, and the SIMPLE algorithm is used to solve the coupled equations of pressure and velocity.

4. RESULTS AND DISCUSSION

4.1. Flame Shape Changes and Development of the Flames. Figure 2 shows the premixed flame propagation process in the duct under different barrier conditions calculated by LES. Figure 2a−c, respectively, shows the premixed flame propagation process at different times in the duct with exactly equal, high to low, and low to high obstacles. It is clear from Figure 2 that at t = 4 ms, the premixed flames in all three figures are spherical flames. As shown in Figure 2a, due to the influence of obstacles, when the premixed flame passed through the first pair of obstacles at 10 ms, the structure of the premixed flame began to wrinkle obviously, and the premixed flame surface began to thin, so that it could pass through the gap between obstacles. When it passed through the second pair of obstacles at 14 ms, the premixed flame began to curl backward, and an obvious symmetrical structure appeared. The symmetrical structure of the flame still existed as the flame passed through the six pairs of obstacles in turn.

In Figure 2a, it can be clearly seen that the flame propagation velocity increases with the increase in the number of obstacles, indicating that the influence of the number of obstacles on the flame velocity is superimposed. Figure 2b,c has similar flame structures to those in (a); the premixed flame passes through the obstacles in turn, and the speed of the premixed flame is gradually accelerated with the increase in the number of obstacles. It can be seen from these two figures that the thickness of the flame surface is determined by the length of the obstacle. The longer the obstacle is, the thinner the flame surface is and vice versa. As can be seen from the structure at different times in Figure 2a−c, the longer the obstacle is, the narrower the obstacle gap is, and the increased pressure on the flame leads to the gradual acceleration of the premixed flame speed.

4.2. Premixed Flame Structure and Flame Front Position. As can be seen from Figure 3, the time of the position of the flame front and the evolution of the flame shape in the numerical simulation have a certain influence for the calculation model using different obstacles. The position of the flame leading edge is determined by measuring the maximum axial distance between the flame leading edge and the leftmost of the duct. First, the premixed flame is not disturbed by obstacles, and the premixed flame is in the laminar flow propagation stage. Because it is not affected by obstacles and side walls of the pipeline, the flame front propagates forward in a spherical manner. After that, the side walls of the duct begins to block the free development of the flame, and the shape of the flame changes from ball- to finger-shaped. Then, due to the interference of obstacles, the premixed flame started to bend and deform through obstacles, and the turbulent flame and laminar flame would be converted, which resulted in the propagation velocity of the premixed flame and the rapid growth of the premixed flame area and the increase in combustion velocity and the heat release rate. When the premixed flame passed through the obstacle for the first time, the front end of the flame takes the shape of a mushroom. After passing through the second pair of obstacles, the “mushroom”-shaped flame begins to break up. It is worth noting that the “mushroom”-shaped part near the upper and lower walls begins to propagate back and begins to reverse through the obstacle hole. In terms of the flame morphology, the premixed flame in the duct under the barrier conditions underwent the transition from layer to turbulent combustion.

Figure 3 also shows that when the obstacle gradually rises from left to right, the time required for the premixed flame to propagate out of the duct is the longest, indicating that the flame propagation velocity is inhibited. The main reason for this result is that the increase in the premixed flame area is relatively small compared with the other two obstacles, resulting in a slower speed increase.

Figure 4 displays that the different obstacles have a great influence on the time evolution of the position of the premixed flame front simulated. The position of the flame front is taken by measuring the maximum axial distance of the premixed flame front from the ignition. As can be seen from Figure 4, the propagation trend of the flame front is the same in the duct with three different obstacles, and the slope of the flame front curve is relatively small at the beginning and becomes larger at the later stage. When the height of the obstacles is equal, the front of the flame spreads out to the right of the pipeline at the shortest time t = 17.8 ms, and when the height of the obstacles is lower and lower from left to right, the transmitting time of the premixed flame is prolonged; when t = 21.0 ms, the flame passed through the rightmost end of the duct. In the third obstruction duct, the obstacle is arranged from left to right at a higher and higher height, it takes the longest time for the premixed flame front to flow out of the rightmost end of the calculation duct.
4.3. Premixed Flame Front Position. Figure 5 shows the change in the front-end velocity of the premixed gas explosion flame with time under three different obstacles. The flame front velocity, \( v \), is calculated as eq 18

\[
v = \frac{\Delta x}{\Delta t}
\]  

(18)

The flame front position, \( x \), is the maximum distance between the flame front at the axis of the tube and the ignition position. \( \Delta x \) is the displacement of the flame front, and \( \Delta t \) is the time it takes for this displacement to occur.

It can be seen from Figure 5 that the velocity of the flame inside the chamber with an obstacle of equal height experienced three oscillations and then rebounded, and the velocity change was the most obvious among the three different obstacles. Also, when the height of the obstacles is lower and lower from left to right, the speed of the initial premixed flame increases slowly, and there were also several small velocity oscillations in the middle of the flame propagation. In the third obstacle duct, where the obstacle is arranged from left to right at a higher and higher height, there was an obvious inhibition effect on velocity of the early premixed flame front.

As can be seen from Figure 5, these three velocity curves all have different degrees of acceleration and deceleration, thus forming velocity oscillation. This is mainly because when the premixed flame front approached the first pair of obstacles, the premixed flame propagation was blocked, leading to the decrease in the flame speed; when the flame passed through the obstacles, the shape of the premixed flame changed from a hemispheric shape to a mushroom shape, and the area of the flame increased significantly, leading to a rapid increase in the flame speed. On passing through the obstacles, the premixed flame exhibits an obvious breaking phenomenon. In addition, it can also be observed that when the flame front propagates through the obstruction, a part of the unburned premixed gas remains in the cavity formed by the obstruction and the inner wall of the duct. Studies in the literature 18,39 show that this part of the unburned premixed gas is closely related to the oscillation in the post-explosion.

4.4. Overpressure Dynamics. Figure 6 shows the variation of LES explosion overpressure with time. Combined with Figure 3, the development trend of the simulated

![Figure 4. Position of the flame front vs time at different obstacles.](image)

![Figure 5. Variation of flame front speed vs with time at different obstacles.](image)

![Figure 6. Development of overpressure at different obstacles, (a) effect of the maximum overpressure and (b) trend of the overpressure.](image)
overpressure is analyzed. It can be seen from Figure 6b that the overpressure inside the duct can be divided into three stages. In the first stage, the explosion overpressure rises gently, and the corresponding change range of the flame propagation speed and flame area is also small. At this time, the premixed flame is not disturbed by premixed obstacles, and the premixed flame is in the laminar flow propagation stage. The flame follows laminar flow propagation, with a small flame surface area and slow rise rate of overpressure. In the second stage, due to the disturbance of the obstacle, the premixed flame passes through the obstacle, and the flame curls and deforms, and the laminar flame transforms to the turbulent flame, resulting in the rapid increase in the premixed flame propagation speed and premixed flame area and the increase in the combustion rate and heat release rate, and the overpressure starts to rise sharply until the front end of the premixed flame bursts out of the right end of the duct. In the third stage, when the front end of the premixed flame rushed out of the duct, the overpressure oscillated significantly, and the overpressure increased first and then decreased. The reason for this phenomenon may be that as the premixed flame rushed out of the duct, the premixed flame gradually went out, and the area of the premixed flame
maintained a rising trend in a short time and then dropped sharply. With the change in the premixed flame area, a Helmholtz oscillation with decreasing amplitude occurs in the apparatus, and the explosion overpressure shows a trend of oscillation and decline and forms several overpressure peaks, among which the medium overpressure peak in the oscillation period corresponds to the maximum premixed flame area peak.

It can be seen from Figure 6a that the change in the height of the obstacles has an obvious effect on the maximum overpressure. When the height of obstacles is equal, the maximum overpressure in the tube is $p = 256.45$ mbar. When the height of the obstacles is lower and lower from left to right, the maximum overpressure in the tube is smaller than in the first, and there were also several small overpressure oscillations in the middle of the flame propagation. In the third kind of obstacle duct, where the obstacle is arranged from left to right at a higher and higher height, there was an obvious inhibition effect on the maximum overpressure in the duct; the maximum overpressure in the tube $p = 38.51$ mbar.

4.5. Flame Speed and Overpressure Dynamics.

Overpressure is an important explosive parameter in the process of premixed gas explosion. Figure 7 displays the coupling relationship between its evolution and flame propagation. The fluctuation of the flame velocity curve is little later than the fluctuation of the pressure curve before the flame front end comes out of the right side of the simulated duct. Overall, the velocity and overpressure curves have the same trend in the early stage. The main reason is that the compression wave is generated on the surface of the flame. When the front end of the flame is about to reach the first pair of obstacles, the propagation of the premixed flame is blocked, and the forward propagation of the compression wave is also blocked by the obstacles, leading to fluctuations. As can be seen from Figure 8, at $t = 4$ ms, the flame propagates rapidly to the first pair of obstacles, while the overpressure wave has passed through the second pair of obstacles. This is also the reason why the overpressure wave appears disturbed earlier than the flame. From the abovementioned analysis, it can be seen that the coupling relationship between explosion overpressure and flame propagation velocity of the premixed gas in the process of pressure-relief explosion in the barrier pipeline is obvious, and the variation trend of the two has a good consistency.

4.6. Flame Shape Changes the Flow Field Structure and Overpressure Cloud.

In order to deeply analyze the premixed flame structure changes of premixed CH$_4$/air explosion under the condition of barriers, after verifying the effectiveness of LES, the overpressure contours and flow field structure of various stages of premixed flame development were obtained through LES, which were compared with the structure of the premixed flame to further reveal the interaction between the pressure wave of the flame structure and flow field in Figure 8. As shown in Figure 8, when $t = 10$ ms, when the premixed flame passed through the first obstacle, the pressure wave in the front of the flame has propagated to the second obstacle. Due to the obstruction by the obstacle, the pressure wave propagates downstream of the obstacle and is greatly reduced, so a low-pressure region with decreasing pressure is formed downstream of the first obstacle, forming a large pressure gradient. At the same time, due to the propagation of the pressure wave, the unburned premixed gas is promoted to propagate rightward at a high speed, and the downstream area of the obstacle is less affected by the pressure wave, resulting in a large velocity gradient, and finally, the gas vortex area is generated downstream of the obstacle. The premixed flow in the duct is in a laminar state, and the intensity of flow field is small, streamline shape rules, basic flow field direction to keep from the ignition end to the end of the duct. Then, the flame front passes over the first pair of obstacles. Due to the large velocity gradient downstream of the obstacles and the accessibility area and the flame front stretches to the sides, the high-temperature and low-density combustion flows into the low-temperature and high-density unburned premixed gas. Under the action of Helmholtz and Rayleigh–Taylor instability, the flame front exhibits folds. When $t = 14$ ms, the flame front propagates to the second obstacle, and the pressure wave has passed the fourth obstacle and propagated to the right, and an obvious low-pressure circular area is formed downstream of the two pairs of obstacles, and an obvious velocity vortex is formed around this circular area by the unburned premixed gas. At the downstream of the first pair of obstacles, the premixed flame front gradually curls under the entrapment of unburned premixed gas vortexes, and folds are generated to form a weak turbulent flame. At this time, the flame surface area increases sharply, the combustion rate accelerates, and the pressure wave also strengthens. When $t = 16$ ms, the flame front passes through the third pair of obstacles and rapidly expands to both sides in a "brush shape". At this time, the overpressure wave has spread to the sixth pair of obstacles, but it can be seen that the low-pressure area downstream of the second and third pairs of obstacles still does not disappear, and there is still an obvious velocity vortex around the low-pressure area.

At the same time, with the increase in the intensity of the flow field, the vortex becomes more obvious, and the effect of the crimping on the gas is obviously enhanced. Thus, the exchange rate between the flammable and unburned premixed gases is increased, which in turn increases the combustion rate and flame propagation speed. Therefore, under the induction of the abovementioned positive excitation effects of flame propagation and flow field, the shape of the premixed flame is seriously deformed, and the intensity of the flow field in the flame front increases sharply.

5. CONCLUSIONS

In this paper, the propagation of methane/air flames in a semi-open pipe with different heights of obstacles is studied using the method of three-dimensional large eddy numerical simulation. The shape of the premixed flame, flow field structure, and overpressure characteristics of the interaction between the flame and the obstacle are simulated accurately in three ducts with obstacles of different heights.

1. The obstacles induce the formation of a flow field area with high turbulence in the pipeline, resulting in the folding and bending deformation of the flame, increasing the flame area and accelerating the flame propagation.

2. Through comparative analysis of the explosion overpressure, the flame propagation speed and the evolution law of the fire area were found to interlink closely and show significant coupling and the tendency is changing with time and there is a high degree of consistency.

3. Due to the obstruction by the obstacle, the overpressure wave propagates to the downstream of the obstacle and is greatly reduced, so a low-overpressure region with decreasing overpressure is formed downstream of the
first obstacle, forming a large pressure gradient. At the same time, due to the effect of obstacles of different heights on flame propagation, the maximum over-pressure in the tube is obviously affected.

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Notes
The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The work is financially supported by the National Natural Science Foundation of China.

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