Simulation of the influence of structural parameters on methane explosion in closed vessels

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Abstract: The gas explosion parameters are affected by the structural parameters. Therefore, the paper numerically studied the gas explosion in cylinder to quantify the dependency of gas explosion parameters on the structural parameters. The results show that both the volume and length-diameter ratio of the cylindrical container affected the methane explosion characteristic parameters. With the increase of volume in the same shape, the time to reach the maximum gas explosion pressure increased, while the maximum rate of pressure rise reduced. With the length-diameter ratio increased, the time to reach the maximum gas explosion pressure became longer and the maximum rate of pressure rise decreased. It is found that the maximum rate of pressure rise conformed to exponential 2D with the volume and length-diameter ratio.

1. Introduction

In the actual industry, the production, transportation and forth putting of combustible gas, disaster accidents are often accompanied. The containers are indispensable storage device in industrial production. When flammable gas disasters occur in the containers of different shapes and volumes, there will be unacceptable consequences due to the size effect [1].

Scholars at home and abroad have done a lot of research on the explosion characteristics of flammable gas in different containers. Wei et al. studied the explosion processes of four 20L vessels with different shapes in order to discuss the change of explosion pressure load and the different of flame behavior in confined space, and found that the pressure time-sequence curves of tubes were more complex, with the appearance of pressure oscillation, and the frequency of oscillation decreased with the increase of length-diameter ratio [2]. Codina et al. investigated the deflagration of stoichiometric ethylene-air mixtures without or with additives (Ar, N2 or CO2) in spherical and cylinder closed vessel with central ignition in order to determine the maximum rates of pressure rise and the deflagration indices, strongly influenced by the length to diameter ratio [3]. Christian et al. studied several influence parameters of deflagrations in closed pipes, and found that with increasing L/D, the explosion pressure decreased and the flame velocity increase [4]. Wang et al. investigated the scale and geometrical features of the prescribed airways through CFD, and found that detonations are more likely to occur when an airway has a larger length-diameter ratio and Flame development is hindered by the wall [5]. Li et al. carried out an experimental study on the propagation characteristics of gas explosion with different length-diameter ratio, such as 1.5, 2.5 and 4. It was found that the ability of cavity reducing flame front is positively associated with the length-diameter ratio [6]. Manju studied the effects of different sizes and shapes of vessels to explosion pressure measurement [7]. These studies are mainly focused on spherical...
containers. There are few studies on the size effect of gas explosions in cylindrical containers, especially the explosion characteristics of cylindrical containers of different sizes.

In view of this, this article intends to study the size effect of methane explosions under larger vessels by changing the volume, pipe length, and inner diameter of larger cylindrical vessels and pipelines, so as to better prevent explosion accidents in pipelines and vessels.

2. Mathematical models and numerical methods
Fluid Simulation Software-Fluent was used for numerical simulation in this paper. The Pressure-Based model, standard k-epsilon model, Species Transport and Finite-Rate combustion model are the main models involved in gas explosion.

The governing equation includes mass conservation equation, momentum conservation equation, energy conservation equation and component equation:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} \tag{2}
\]

\(\sigma_{ij}\) is stress tensor,

\[
\sigma_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_i} \delta_{ij} + \frac{\partial (\rho u_i)}{\partial x_i} \tag{3}
\]

\[
\frac{\partial (\rho e)}{\partial t} + \frac{\partial (\rho u_i e + p)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho \frac{k}{\partial x_i} - \sum h_m J_m + u_j \sigma_{ij} \right) + \dot{Q}_c \tag{4}
\]

\[
\frac{\partial (\rho Y_m)}{\partial t} + \frac{\partial (\rho u_i Y_m)}{\partial x_i} = -\frac{\partial (\rho D_m \frac{\partial Y_m}{\partial x_i})}{\partial x_i} + \omega_m \tag{5}
\]

Where \(\rho\) is density, \(t\) is time, \(u_i\) is velocity, \(p\) is pressure, \(\mu\) is viscosity, \(k\) is thermal conductivity, \(T\) is temperature. \(e = -p/\rho + u_i^2/2\) is internal energy, \(\dot{Q}_c\) is chemical reaction source. \(Y_m, D_m, h_m, \omega_m\) are specie \(m\)'s the mass fraction, mass diffusion coefficient, \(c_p\), diffusion flux and chemical reaction rate. Arrhenius combustion rate is formulated as the combustion model:

\[
R_{f_{ul}} = B \beta R T Y Z e \exp \left( -\frac{E}{RT} \right) \tag{6}
\]

Where \(B\) is pre-exponential factor, \(E\) is activation energy for the reaction, \(R\) is universal gas constant, \(R_{f_{ul}}\) is forward rate constant for reaction of Arrhenius, \(\beta R\) is temperature exponent.

The models adopted in this paper include cylindrical containers with different aspect ratio of 4L, 10L, 33L, 80L, 268L. The mesh used structured grids, and the average mesh quality is above 0.99. Methane-air is in a static state closed to ambient initial pressure and temperature the mass concentration of methane is 0.051, and the mass concentration of oxygen content is 0.23. The ignition source is a high-temperature ignition zone with a radius of 2cm and a temperature of 2000K set at the center of the container. Without considering the heat dissipation, one-step reaction is adopted, and adiabatic non-slip of the wall is considered. By comparing the maximum explosion pressure of vessels of different volumes obtained through experiments and simulations\(^7,\ 8\), the results are shown in Figure 1 to verify the correctness of the simulation.
3. Results and Discussion

The effects of different volume and different aspect ratio on deflagration characteristics of cylindrical vessels were studied. In this paper, cylindrical containers with aspect ratios of 1, 2, 4 and 8 with volumes of 4L, 10L, 33L, 80L and 268L are selected to discuss the effects of the volume-aspect ratio on the explosion time and pressure rise rate of cylindrical containers.

For cylinders with different volumes and different aspect ratios, the explosion pressure is basically the same in the same initial state, as shown in Figure 2. The explosion time of methane in cylindrical containers with different volumes and aspect ratios is shown in Table 1. It is found that the explosion time is positively correlated with the volume and aspect ratio of cylindrical containers.

| L/D | Volume (L) | 1    | 2    | 4     | 8     |
|-----|------------|------|------|-------|-------|
| 4   | 5.965      | 6.314| 9.45 | 17.57 |
| 10  | 7.824      | 9.06 | 12.75| 23.83 |
| 33  | 15.765     | 17.4 | 25.27| 43.19 |
| 80  | 23.47      | 28.86| 40.43| 72.43 |
| 268 | 37.97      | 45.52| 61.12| 103.1 |

For cylindrical containers with the same aspect ratio, the growth rate of explosion time first increases and then decreases with the increase of volume, indicating that the impact of volume is more obvious
when the volume is small. The impact curve of volume and explosion time is shown in Figure 3. For the same volume of the cylindrical container, explosion time positively correlated with the aspect ratio, with aspect ratio increases, the amplitude of explosion growth also gradually become fast. It can be seen from Table 1 that when the volume is 4L, the explosion time difference between the aspect ratio 1 and 8 is 11.61ms, and when the volume is 268L, the difference between the two reaches 65.13ms. It can be found from Figure 3 that when the volume is fixed, the explosion characteristics of the cylinder is positively correlated with the impact of the aspect ratio. And the effect of the volume under cylindrical container with large aspect ratio on the explosion time is more obvious. When the aspect ratio is 1, the explosion time difference between volume 4L and volume 268L is 32.01ms; when the length-diameter ratio is 8, the explosion time difference is 85.53ms. This indicates that the explosion time will increase with the increase of aspect ratio, which is because the flame development in the container with large aspect ratio is hindered by the cylindrical wall and consumes more kinetic energy\[9\].

![Figure 3. The effect of volume and L/D to the time to reach P_max in Cylindrical vessels](image)

The maximum pressure rise rate of cylindrical vessels of different volumes and aspect ratios were studied. As shown in Figure 4, the pressure rise rate is negatively correlated with the volume of the cylindrical vessel. With the increase of the volume, the maximum pressure rise rate begins to decrease. It is found that the higher the length-diameter ratio is, the lower the maximum pressure rise rate is. This is because the length-diameter ratio is larger, the explosion time is longer and the pressure rise rate is slower.

![Figure 4. The effect of volume and L/D to maximum pressure rise in Cylindrical vessels volume](image)
Figure 5. The influence of L/D and volume on the maximum pressure rise rate of cylindrical vessel

It is found that both aspect ratio and volume affect the deflagration characteristics of cylindrical vessels. In the same initial case, it is found that cylindrical containers with different aspect ratios and different volumes conform to exponential 2D by just taking into account the container factors, including different length to diameter ratio and different volume. The fitting result basically conforms to the function 7, according to the Figure 5, and coefficient of determination reaches 0.94857.

\[
\left( \frac{dp}{dt} \right)_{max} = -977.48 + 6553.438 \exp \left( -\frac{V}{251.938} \right) \times \exp \left( -\frac{L/D}{8.06} \right)
\]  

(7)

4. Conclusion

The explosion time and the maximum pressure rise rate change with the volume. When the container volume increases, the explosion time of combustible gas in the container becomes longer, the maximum pressure rise rate decreases, and the explosion pressure is basically the same. Ideally, the pressure of gas is only related to the initial and terminal states of the explosion. For cylindrical vessels with different aspect ratios, with the increase of volume, the explosion time increases and the maximum pressure rise rate decreases. The aspect ratio and volume of cylindrical vessels together affect the explosion characteristics of combustible gas. The larger the aspect ratio is, the smaller the maximum pressure rise rate is. The increase of aspect ratio inhibited pressure rise rate. As the volume increases, the influence of volume on the maximum pressure rise rate becomes more and more weakened.

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