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Influence of geometrical shapes on unconfined vapor cloud explosion

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ABSTRACT

The vapor cloud explosion (VCE) usually results in large financial and environmental damages. There are many methods to evaluate the consequences of VCE and one of them is the TNO Multi-Energy method (MEM). In the practical applications, the MEM has some weaknesses. For example, it is assumed that the explosion model is hemispherical, which is usually inconsistent with the actual situations. In order to examine the effect of the geometrical shapes on explosion characteristics, a constant volume of clouds with different height-width ratios and length-width ratios were studied. For the vapor cloud with a given volume (32 m^3), the geometrical shapes have a great influence on the explosion overpressure, but little on the explosion temperature. When the height-width ratio is 0.5 (the corresponding geometrical shape is 4 m × 4 m × 2 m), the explosion peak overpressure reaches the maximum of 1.57 bar, which is 3.6 times of that (0.44 bar) for the 2 m × 2 m × 8 m vapor cloud. For a constant volume of clouds with the four different height-width ratios in this paper, the MEM predictions correspond to three different initial explosion strengths. As effect of the geometrical shapes on the vapor cloud explosion was not taken into account in the MEM, its predicted results have a greater deviation, especially in the far field. For the scenarios calculated in this study, the relative error for the explosion overpressure predicated in the MEM reaches 150%.

1. Introduction

During the transport, storage, processing and use of flammable gases, a vapor cloud explosion (VCE) may occur if the flammable gas and air mixture formed by their leakage to the atmosphere is accidentally ignited. The VCE is defined as "an explosion resulting from an ignition of a premixed cloud of flammable vapor, gas or spray with air, in which flames accelerate to sufficiently high velocities to produce significant overpressure" (Mercx and van den Berg, 2005). The VCE usually results in large financial and environmental damages in addition to potential injury and loss of life (Mannan et al., 2002). For example, in November 22, 2013, a crude oil leaking explosion occurred in Qingdao, China. 62 people were killed and 136 others were injured during the accident. Besides, the direct property losses reached up to 0.1 billion US dollars (Zhu et al., 2015).

Some analytical methods was used to study the explosion effect of vapor clouds. Fishburn et al. (1981) studied the blast pressures from a pancake shaped fuel-air cloud detonation. The theoretical C-J detonation pressure was directly used to indicate the overpressure inside the vapor cloud. They concluded that the cloud shape effectively keeps the force of the explosion near the ground. Pickles and Bittleston (1983) calculated the blast pressures of the asymmetrical blast for an ellipsoidal and a cigar-shaped cloud with ignition at one end. A linearized acoustic approximation was used. The calculation was done with the assumption that the cloud expands primarily in the directions normal to its long axis. They concluded that the overpressure generated from a hemispherical gas cloud is the greatest. Paul (1985) also calculated the deflagration overpressure of an elongated vapor cloud with ignition at one end. He used the linear acoustic theory, too. He found that the overpressures for an elongated cloud are significantly lower than the hemispherical cloud. Many idealized assumptions were used in these analytical methods, and there are some limitations in predicting the actual explosion effect.

For vapor cloud explosions, the trinitrotoluene (TNT) equivalent method was generally used in the calculation of the specific distance by predicting the overpressure decay according to the distance from the gas explosion site (Bjerketvedt et al., 1997). However, the TNT equivalent method is a very conservative method because it always assumes that a detonation shock wave occurs when a gas explosion at the stoichiometry condition happens (Kang et al., 2017). On the basis of the TNT equivalent method, Van den Berg (1985) proposed the TNO Multi-Energy method (MEM). The MEM classifies the peak overpressure at the center region of the gas explosion into 10 classes using an empirical correlation, and as a result, the overpressure decay according to the distance from the gas explosion region can be predicted differently depending on the class. Nevertheless, like the TNT equivalent method,

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the MEM also has some weaknesses. For example, it is assumed that the gas explosion occurs in the case of hemispherical with a steady flame speed, and the chemical reactions occur under stoichiometric conditions. But these assumptions are too idealistic, and there are some limitations in predicting the actual explosion source strength or dynamics. In order to compensate for the shortcomings of the above methods, and predict the hazards of vapor cloud explosion more accurately, it is necessary to use computational fluid dynamics (CFD) method (Qiao and Zhang, 2010). The use of CFD has many advantages, including more precise estimates of the energy and resulting pressure of the blast wave, as well as the ability to evaluate non-symmetrical effects caused by realistic geometries, gas cloud variations and ignition locations (Hansen et al., 2010).

In the application of CFD method to study the VCE, a lot of research have been done (Hughes et al., 2001; Leyer et al., 1993; Tauseef et al., 2011). Most of previous investigations mainly focused on the gas cloud size, the development of turbulence during the explosion (Kim et al., 2014; Tomizuka et al., 2013; Ma et al., 2014) and the subsequent blast propagation (Puttock et al., 2000; Tufano et al., 1998; Hansen et al., 2013). The literature on how objects can significantly influence the dynamics of the blast wave were also available (Li et al., 2014, 2016; Cong and Bi, 2008) But hazards for a vapor cloud with geometrical shapes have received relatively little attention.

During the process of consequences prediction for a vapor cloud explosion, the geometrical shape of the cloud is usually assumed to be hemispherical. For the combustible vapor cloud of same volume, the hemispherical cloud has the highest explosion intensity (Bjerketvedt et al., 1997). The results predicted using the hemispherical model are usually safe and conservative in engineering applications. But the hemispherical vapor cloud is usually inconsistent with the actual situations. For example, if a flammable liquid leak occurred, the liquid would spread on the ground firstly, and then formed a vapor cloud with a large bottom and a relatively small height (Epstein and Fauske, 2007). Therefore, it is necessary to study the trend of the explosion characteristics for clouds with geometrical shapes, and analyze the effect of cloud shapes on the consequences of the explosion.

The object of the study was to systematically examine the effect of the geometrical shapes on explosion characteristics in the open space using the computational fluid dynamics software AutoReaGas. The models used in the simulations were a constant volume of clouds with different height-width ratios and length-width ratios. The effect of the geometrical shapes was revealed by comparing the explosion pressure, temperature and flame region at various dimensionless distances and absolute distances, respectively. Meanwhile, the explosion overpressures of clouds with geometrical shapes were also compared with the MEM predictions, and the differences between them were pointed out. This study can provide a reference for the prevention and prediction of the consequences of unconfined vapor cloud explosion accident.

2. Governing equations and computational method

Explosion process of flammable gas was expressed by the following governing equations using the Cartesian tensor notation.

The mass conservation equation is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0 \tag{1}$$

The momentum conservation equation is:

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

The equation of conservation of energy is:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}(\rho u_j E) = \frac{\partial}{\partial x_j}\left(\Gamma_E \frac{\partial E}{\partial x_j}\right) - \frac{\partial}{\partial x_j}(p u_j) + \tau_{ij}\frac{\partial u_i}{\partial x_j} \tag{3}$$

Where x is the space coordinate, t is the time coordinate, ρ is the density, u is the velocity, p is the static pressure, i and j are the coordinate directions; the specific internal energy $E = C_v T + m_{fu} H_c$, C_v is the constant volume specific heat, T is the temperature, m_{fu} is the mass fraction of fuel, H_c is the heat of combustion; the turbulent diffusion coefficient $\Gamma_* = \mu_t / (\sigma)*$, $(\sigma)*$ is the turbulent Prandtl constant, taking the default value; τ_{ij} is the viscous stress tensor, its expression is:

$$\tau_{ij} = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}\left(\rho k + \mu_t \frac{\partial u_i}{\partial x_j}\right) \tag{4}$$

Where the turbulence viscosity coefficient $\mu_t = C_\mu \rho k^2 / \varepsilon$, k, ε is the turbulent kinetic energy and its dissipation rate respective, a model constant $C_\mu = 0.09 m^2 / s$; δ_{ij} is the Kronecker delta.

Turbulence model is described by:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho u_j k) = \frac{\partial}{\partial x_j}\left(\Gamma_k \frac{\partial k}{\partial x_j}\right) + \tau_{ij}\frac{\partial u_i}{\partial x_j} - \rho\varepsilon \tag{5}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(\rho u_j \varepsilon) = \frac{\partial}{\partial x_j}\left(\Gamma_\varepsilon \frac{\partial \varepsilon}{\partial x_j}\right) + C_1 \frac{\varepsilon}{k}\tau_{ij}\frac{\partial u_i}{\partial x_j} - C_2 \frac{\rho \varepsilon^2}{k} \tag{6}$$

Where C_1 and C_2 are the constants.

One-step reaction model describes the combustion process uses of unreacted fuel/air mixture burning, explosion, translating reactants, and releasing quantity of heat. This is mathematically formulated as a conservation equation for the fuel mass fraction:

$$\frac{\partial}{\partial t}(\rho m_{fu}) + \frac{\partial}{\partial x_j}(\rho u_j m_{fu}) = \frac{\partial}{\partial x_j}\left(\Gamma_{fu} \frac{\partial m_{fu}}{\partial x_j}\right) + R_{fu} \tag{7}$$

Where gas combustion rate $R_{fu} = C_t \rho \frac{S_t^2}{\Gamma_{fu}} R_{\min}$, $R_{\min}$ is the minimum value of the fuel mass fraction, the oxygen mass fraction and the mass fraction of the product, C_t is the main adjustable parameters of flame speed constant; the turbulent combustion rate is expressed by:

$$S_t = 1.8 u_t^{0.412} \cdot L_t^{0.196} \cdot S_l^{0.784} \cdot \nu^{-0.196} \tag{8}$$

Where u_t is the turbulence intensity; L_t is the characteristic length size; S_l is the specific laminar burning velocity; ν is the kinematic viscosity of the unburned mixture.

The conservation equations were solved using a finite volume method in the computational code. The computational domain was subdivided into a finite number of rectangular control volumes. The SIMPLE method was taken to solve the pressure-velocity coupling of the momentum conservation equations and the mass balance. One order upwind scheme and adaptive time step were used for solving governing equations. The time step meets following CFL stability criterion:

$$\Delta t = \frac{\omega \cdot \Delta x}{c + |V|} \tag{9}$$

Where ω is the coefficient of time step, taking 1.0 in this simulation; Δx is the maximum element size; c is the sound velocity in calculating cells; V is the velocity vector.

3. Verification of the numerical method

To verify the validity of the numerical method, a simulation was conducted corresponding to the experimental conditions of the MERGE experiment (Mercx, 1994). The MERGE experiments were performed in six different experimental geometrics. In this verification, the MERGE-C experiment with a medium scale of 45 m^3 flammable cloud was chosen. As shown in Fig. 1, all the calculation conditions were similar to the experiment. The 4.5 m × 4.5 m × 2.25 m cuboid cloud was located on the ground surface, filled with stoichiometric methane/air premixed gas. The build-in obstacles with orthogonal arrangement of 10 × 10 × 5 were set up inside the cloud. The diameter of the obstacles was 8.6 cm, and the space between adjacent obstacles was 40 cm. The