Study on Fire Simulation and Safety Distance of Reactor Thermal Runaway

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Abstract: With the development of chemical industry, fire and explosion accidents become more and more frequent. In this paper, a simple analysis is carried out based on the thermal runaway of the reactor, and the explosion simulation is carried out by using the fluent numerical simulation software, according to the standard turbulence model (k-ε) and the component transport selected EDC- (vortex-dissipative) model. Simulation result intuitively show the pressure, temperature, speed and the relationship between the distance from the center of burns. The results show that the pressure, temperature and velocity decrease exponentially after a certain distance away from the explosion center, the relative safe distance is between 50 and 100 meters in the dangerous area within 50 meters, and in the 100-meter outside pressure temperature back to normal for a safe distance.

1. Introduction

In all kinds of chemical plants, accidents are inevitable due to the design and manufacture of the equipment, technical or artificial reasons in the process of using, and the runaway of the reactor. Once the reactor loses control and leaks out of control, if the material is flammable, explosive gas or high-pressure gasified liquid, in the air, there will be extremely rapid chemical reactions, such as open fire, sparks, static electricity, etc., and at the same time, a large amount of energy will be released to the surrounding environment. These energy thermal radiation, shock wave and other forms of diffusion pose a threat to the surrounding personnel and equipment [1]. In terms of explosion limit, a series of achievements have been made abroad earlier than at home. Coward and Jones first put forward the concept of combustible gas and vapor cloud limit explosion. In 1965, the US Mine Administration Zabettak is measured the gas explosion limit by propagation method [2]. In the aspect of shock wave, Lin[3] studied the relationship between flame and shock wave. He confirmed the positive feedback effect of flame and shock wave, and obtained the relationship between flame and shock wave.

In this paper, by means of numerical simulation, the explosion accident of known materials is simulated, and the influence range of fire source on the surrounding environment and equipment is calculated [4]. According to the research in this field at home and abroad, it is determined that the simulation condition is unconfined gas cloud explosion, that is, after the reactor is out of control, the gaseous material leaks into the air to form a uniform gas cloud, and the combustion explosion occurs after the ignition source [5]. Based on the study of real gas cloud explosion, the combustion reaction under confinement [6] is explored. According to the simulation results and data analysis, the range of thermal radiation damage, the change curve, the influence range of shock wave and the change curve are determined, which has certain reference value for the safety distance between the material reactor...
design and installation and the emergency safety rescue distance.

2. Research Task
The combustible gas in the tank (reactor) is liquefied by pressurization. When the tank (reactor) fails and ruptures, part of the liquid combustible gas flashes and changes into gas, which dissipates into the air. After mixing with air, a burst occurs when the ignition source is encountered [7]. Although only part of the gas is ignited for the first time, once the first explosion occurs, the ambient temperature rises rapidly, which can become a new ignition source. The remaining unvaporized liquid in the storage tank (reactor) will also immediately vaporize and burn and explode. This cycle is completed until all combustible gases are completely burned.

In order to obtain more specific results of combustion, the combustion calculation and explosion simulation are carried out under the given conditions, the working conditions are as follows:

The reaction kettle with a volume of 5 cubic meters before the explosion was not filled with material at the time of explosion, and the temperature was 182.2 °C and the pressure was 17.96 bar. At the time of explosion, the following materials were loaded: methanol (CH₄O): 577.236 kg; methyl acetate (C₃H₆O₂): 1338.066 kg; acetic acid (C₂H₄O₂): 1084.704 kg. After the explosion, some of the materials flash and the initial state in the air is as follows: The steam temperature is 79.1 ℃, the volume is 707.665 m³. Under the condition of no air, methanol(CH₄O): 335.1 kg; methyl acetate (C₃H₆O₂): 941.343 kg; acetic acid (C₂H₄O₂): 180.691 kg.

3. Study on Explosion under Specific Working Conditions

3.1 Combustion zone calculation
Assuming that three kinds of materials, methanol (CH₄O), methyl acetate (C₃H₆O₂) and acetic acid (C₂H₄O₂), are completely burned in air, all of them produce water and carbon dioxide after combustion, then the total reaction equation is:

\[ \text{CH}_4\text{O} + \text{C}_3\text{H}_6\text{O}_2 + \text{C}_2\text{H}_4\text{O}_2 + 7\text{O}_2 = 6\text{CO}_2 + 7\text{H}_2\text{O} \]

According to the formula:

\[ V = \frac{G}{\rho} \times \frac{t + 273}{273} \]

Formula V: the volume of combustion generated gas; G: the quality of the combustion gas; P: the density of the gas generated by combustion; t: the temperature of the gas generated. According to the formula:

\[ t = \frac{\Sigma Q_W}{C_W \times W} \]

Q: combustible combustion heat; W: combustible mass C: average specific heat capacity of gas generated, where the default is 1256 J/(kg·K); W: generate gas mass.

Check the relevant information: three kinds of flammable gas combustion value is: methanol (CH₄O): 2.27×10⁷ J/kg; methyl acetate (C₃H₆O₂): 2.153×10⁷ J/kg; acetic acid (C₂H₄O₂): 1.456×10⁷ J/kg. \( \Sigma Q_W=5770.51 \times 10^7 \) J, because the mass of the three kinds of combustible gases is known, it is easy to obtain the total mass of the generated gases: 20732.4 kg.

The temperature of the gas can be calculated according to the known conditions above:

\[ t = \frac{\Sigma Q_W}{C \times W} = \frac{5770.51 \times 10^7}{1256 \times 20372.4} = 2255.18 \]

The average relative molecular weight of the product is 28.66; the density of the product is 1.28 kg / m³. Based on the above data:

\[ V = \frac{G}{\rho} \times \frac{t + 273}{273} = \frac{20372.4}{1.28} \times \frac{273 + 2255.18}{273} = 147393.24 \]

And then we can get the radius is 32.77 meters.

That is, less than 5 cubic meters of combustible liquefied gas combustion, its combustion radius of 32.77 meters, within this distance, all combustible substances are likely to be ignited, personnel are extremely vulnerable to burns.
3.2 Decomposition and Prediction of Simulated Data

3.2.1 Simulation model under working conditions

According to the given working conditions, three kinds of materials, methanol, acetic acid and methyl acetate, are simulated and mixed into the air, and then explosion occurs in the ignition source, and there is no container around them, that is, the simulation of unconstrained explosion. So the following models are set up before the simulation:

![Simulation model](image)

As shown in the above model, B in three kinds of material and air premixed vapor cloud formation, after mixing two kinds of explosive gases to achieve lower explosive limit, set conditions for raw material, ignition source temperature to 1200 K; C is filled with air. The setting conditions are: temperature 300K, pressure 1 standard atmospheric pressure, component: air component. B premixed gas in high temperature points within the fire and explosion, as there is no wall B round, instant temperature and pressure to release, in order to explore the C inside the quantities such as temperature, pressure, component, the speed of change.

3.2.2 Simulation prediction

Vapor cloud explosion is an extremely rapid combustion reaction, releasing a large amount of energy in a very short time. The principle of combustion is similar to that of combustion, all of which need to satisfy the three elements of combustion:

1. combustible

The explosion explains the combustible matter as the combustible / explosive material reaches the explosive limit (LEL), and the following information is obtained from the relevant information.

| Matter         | Flash point/°C | Ignite/°C | Natural point/°C | Low explosive limit/% |
|----------------|----------------|-----------|------------------|-----------------------|
| Methanol       | 12             | -         | 436              | 6                     |
| Acetic acid    | 39             | -         | -                | -                     |
| Methyl acetate | -10            | 454       | -                | 3.1                   |

As each material has its own lower limit of explosion in the air, it is necessary to further analyze and calculate the lower limit of the three materials before the simulation. The total volume of the material is 707.665m without air. The radius of the ball is 5.529m, and the two-dimensional circular area is 95.99m². Each material mass is known, according to the ideal gas standard state equation: PV=nRT, and changing pressure and temperature to 300K, 101kPa. We can get the volume of the corresponding material. The volumes of methanol, acetic acid and methyl acetate are 303.562, 87.285 and 368.698m³. According to the explosive limit equation of mixed gas: \( V=100/(P_1/L_1+P_2/L_2) \), (P is component volume fraction L is the lower limit of component explosion). The lower explosive limit of the mixture is 4.1735%, and calculated according to the volume of detonating gas. The total volume of mixed gas \( V=16952.699m^3 \),
radius $R=15.9388m.$, that is, the radius of B circle in Figure 1 can be set to 16m.

(2) Incendiary source

Methanol and methyl acetate all have flammability and acetic acid is not combustible, so the ignition point of methanol and methyl acetate should only be considered when setting the ignition temperature. As described in Table 1, methyl acetate is flammable at 454 °C, so it is only necessary to set the ignition temperature above 454 °C in the simulation. In this simulation, the ignition temperature is set at 1200 kg. in order to guarantee the energy unit to achieve the effect of explosion, the ignition source is set up in the state of high temperature and high pressure when the ignition source is defined.

(3) Combustion aid

In general, the combustion-supporting material is oxygen in the air. In the simulation process, the oxygen concentration is approximately unchanged after the formation of the premixed vapor cloud, and the numerical value set here does not need to be interfered with artificially.

3.3 Simulation Process Parameter Setting

After multiple simulations, the most selected grid size is 300*300 meters, the cell size is 0.5*0.5 meters, and the center material area circle radius is 16 meters. The model selects the standard turbulence model ($k-\varepsilon$) and opens the energy equation. In multiphase flow and chemical reaction (combustion), the species transport is required to be opened, and the standard volume general method and the EDC model are used. The calculation time step is set to 0.001s.

3.4 Simulation result

After 120 steps of iteration, the minimum residual value can be regarded as convergent. The resulting pressure, temperature, and velocity clouds are as follows:

Figure 2. Temperature, pressure and velocity clouds map
For ease of observation, draw the results as X-Y curves on the center line, as follows:

(a)  
(b)  
(c)  

Figure3. Curves of pressure, temperature and velocity

According to the figure, we can get the following analysis:

(1) Pressure
The maximum explosion pressure is 6.57e+7 Pa. It decreases exponentially after a certain distance away from the center, and the pressure drops to the standard atmospheric pressure after 100 meters from the explosion source, that is, the diameter of the explosion is about 100 meters.

(2) Temperature
The temperature in the center of the explosion source reaches a maximum of 5000k. After a certain distance away from the center, it decreases exponentially. After about 35 meters from the source, the temperature begins to decrease. After 100 meters away from the center, the temperature drops to the normal ambient temperature.

(3) Velocity
The maximum velocity of the gas produced by the explosion is as high as 7289 m/s. After 15 meters from the detonation source, the velocity starts to decrease by 100 meters and there is almost no movement of the gas.

Many scholars at home and abroad have done experimental research on the damage of shock wave to human beings. The research shows that shock wave can be divided into two kinds of damage, one is the direct action of shock wave, the other is indirect action of shock wave. Because the explosion under unconstrained conditions is simulated in this paper, the direct action of shock wave is mainly considered. See the table below:
Table 2. Overpressure injury

| Overpressure (MPa) | extent of injury |
|-------------------|------------------|
| < 0.02            | safe             |
| 0.2~0.3           | light            |
| 0.3~0.5           | secondary        |
| 0.5~1.0           | serious          |
| > 1.0             | Extremely serious|

By analysis, it is found that the most serious area is within 20 meters and the area of moderate injury is serious, and the area of moderate injury is a safe area beyond 100 meters.

4. Conclusion
In this paper, the model of explosion accident caused by the leakage of methanol, methyl acetate and acetic acid into air is analyzed, and the pressure, temperature and velocity changes under given working conditions are calculated by Fluent. It provides theoretical basis for accident rescue, emergency relief and safe evacuation. Through the above analysis, the main conclusions are as follows:

(1) To avoid leakage, fire and explosion, it is essential to prevent leakage. It is necessary to do a good job in the safety of the device, pay attention to maintenance, use and scrap according to the regulations.

(2) All sources of fire are strictly prohibited in the production area. Ignition sources may include chemical fire sources, impact fire sources, electrical fire sources, high temperature fire sources, etc. If there is no ignition source, even in case of leakage, it can be dealt with in time.

(3) According to the analysis of the simulation results, within the range of 50 meters from the explosion source, because of the production of high temperature, high pressure and high speed fluids, it is an absolute dangerous area. Within 100 meters, the temperature, pressure, and velocity of flow begin to decrease, which is beyond the relative dangerous area of 100 meters. Temperature, pressure, and velocity are almost normal and are therefore relatively safe. In the event of this fire and explosion accident, rescue and disaster relief must be within 50 meters and safe evacuation within 100 meters.

Acknowledgements
First of all, I would like to thank my senior for the guidance, secondly, I would like to thank myself for my hard study, and finally I would like to thank my tutor for the advice

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