Numerical simulation of toxic gas diffusion in confined space

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Abstract. In this paper, the numerical simulation method is used to study the gas diffusion in a limited space under the scene of poisonous gas attack or leakage. Based on the STAR-CCM + software, the toxic gas diffusion process in a limited enclosed space under specific flow field conditions was simulated and analyzed, and the effects of different wind speeds on the diffusion law and concentration field distribution were studied.

1. Introduction
The study on the diffusion of toxic gases mainly considers two scenarios: terrorist attacks and chemical spills. The regional situation is tense, and frictions caused by ethnic and religious contradictions occur from time to time. With economic development and urbanization, public places with high traffic density have become important targets for terrorist attacks. There are a large number of chemical dangerous goods and dangerous and harmful gases in the metal and chemical industries. Once an accident occurs, the toxic gas diffuses in the atmosphere, which is likely to cause a large number of casualties and large-scale environmental pollution in a short time [1]. At present, the research methods on the evolution of toxic gas include three types: numerical simulation, field test and wind tunnel test. Computer numerical simulation has the advantages of safety, low cost, high repeatability, and the ability to simulate the effect of a single influencing factor. It can describe the spatial and temporal distribution of three-dimensional flow fields and pollutants in detail [2, 3].

Taking into account the feasibility of subsequent experimental verification, this paper will use absolute ethanol as the diffusion medium and perform numerical simulation based on STAR-CCM + software to study its diffusion law and the influence of different flow field environments. By studying the law of toxic gas diffusion, the scope of hazards caused by toxic substances can be calculated quickly and accurately, providing important scientific guidance for the efficient realization of personnel evacuation and decontamination [4].

2. Model establishment

2.1. Basic governing equation
The law of the flow field formed after the toxic and dangerous gas is instantaneously released in a confined space generally meets the basic fluid mechanics equations described by the Navier-Stokes equations (NS equations), namely the mass conservation equation, momentum conservation equation, and energy conservation equation. In the description of turbulent flow, the system of equations is Reynolds approximation, and the equations are used to close the system of equations [5].
Basic assumptions:
  a) The gas in the confined space is treated as an incompressible fluid, and it is in a turbulent state;
  b) The mixed gas of air and volatile ethanol is regarded as an ideal gas, which follows the ideal gas equation of state, and no chemical reaction occurs during the convection diffusion process;
  c) During the gas diffusion process, the temperature does not change, and the heat transfer between gases is not considered;
  d) The rate of ethanol volatilization does not change during the diffusion process.

Based on the above assumptions, we believe that the diffusion of gases in confined spaces is a single-phase diffusion problem without chemical reactions [6].

1) Mass conservation equation (Continuity equation)

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \]  

(1)

Where \( \rho \) is the fluid density, and \( u_j (j=1, 2, 3) \) is the velocity in three directions.

2) Momentum conservation equation

\[ \frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\mu \frac{\partial u_i}{\partial x_j}) + (\rho - \rho_a) g_i \]  

(2)

Where \( \mu \) is the dynamic viscosity of the fluid, \( g \) is the acceleration of gravity, \( p \) is the absolute pressure, and \( \rho_a \) is the density of air.

3) Energy conservation equation

\[ \frac{\partial (\rho T)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j T) = \frac{\partial}{\partial x_j} \left( \frac{k}{c_p} \frac{\partial u_j}{\partial x_j} \right) + S_f \]  

(3)

Where \( c_p \) is the specific heat capacity, \( T \) is the temperature, \( k \) is the fluid heat transfer coefficient, and \( S_f \) is the viscous dissipation term.

4) Diffusion equation

\[ \frac{\partial (C)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = \frac{\partial}{\partial x_j} \left[ D \frac{\partial (\rho C)}{\partial x_j} \right] \]  

(4)

Where \( C \) is the toxic gas concentration and \( D \) is the turbulent diffusion coefficient.

2.2. Physical Model and Meshing

As shown in Figure 1, a three-dimensional physical model is built using the module that comes with STAR-CCM + software, and the solution area is meshed. The size of the limited space structure is, and the number of grids is about 127,000.
2.3. Boundary conditions and solution method settings
This article studies the diffusion of anhydrous ethanol in a confined space. The ethanol evaporation rate is set to 7g / s, the inlet air velocity on the left wall is 0.5m / s or 1m / s, and the right side is the pressure outlet. The location of the poison gas source is considered as shown in Figure 2, there are four cases, the position coordinate points are A(0.2, 0, 0.2), B (0.2, 0.0.75), C (1.4, 0, 0.2), D (1.4, 0.0.75) (unit: m).

In the simulation calculation, an implicit unsteady, standard K-Epsilon turbulence model is used, and the time step of the iteration is taken as 0.5s. At the same time, several solving sections are set. The concentration distribution and velocity distribution map are saved every 10s in physical time and total diffusion time is 2min.

3. Simulation results and analysis
3.1. Analysis of diffusion law
With the small fan on the left wall fully open and the poisonous gas source located at coordinates (0.2, 0, and 0.2) as the basic flow field, the diffusion of poisonous gas in this space is discussed. By comparing the concentration distribution maps of the sections x = 0.8m, x = 1.4m, and x = 2.0m at intervals of 10s, it is found that the diffusion rules of the sections in the direction of the inlet air velocity are basically
the same, which is about far from the source of the release, and overall The smaller the ethanol concentration, the slightly delayed the diffusion process, and the flow field morphology was basically stable in about 70s. Take wind speed $v = 1\, \text{m/s}$ as an example,

As shown in Figures 3 and 4, the volatile ethanol gas gradually diffused upward from the ground release source and diffused toward the wind speed of the side. Due to the height limitation of the space, ethanol accumulated on the upper top surface, and then diffused back and forth to form an obvious Turbulence.

![Figure 3. Distribution chart of ethanol concentration at $x = 1.4\, \text{m}$ cross section](image)

![Figure 4. Distribution chart of ethanol concentration at $z = 0.75\, \text{m}$ cross section](image)

3.2. Influence of wind speed on diffusion

Figure 5 shows the velocity vector diagram at the same time when the wind speed $v = 0.5\, \text{m/s}$ and $V = 1\, \text{m/s}$ at $x = 0.2\, \text{m}$ and $z = 0.75\, \text{m}$, respectively. It can be seen that the change of wind speed has a significant impact on the velocity distribution of the whole flow field.
Analysis and comparison of the distribution of ethanol concentration on three different dimensional cross sections after the same time spread under the conditions of wind speed $v = 0.5\, \text{m/s}$ (left) and $v = 1\, \text{m/s}$ (right), we can find:

1) The larger the wind speed, the faster the gas diffuses downward in the wind direction, the longer the distance, and the larger the diffusion area.

2) When the wind speed is small, the trend of ethanol diffusion is more uniform, and when the wind speed is large, a clear diffusion phenomenon from the side wall to the middle appears. It may be speculated that the greater the wind speed in the confined space, the greater the external force driving the toxic gas diffusion, which accelerates and enhances the formation of turbulence, so the vortex return is more obvious. The figure 6 below only uses the time $t = 100\, \text{s}$ as an example.

Figure 5. Velocity vector diagram

Figure 6. Comparison of concentration distribution on the same section at different wind speeds
4. Conclusion
The wind speed of the flow field is an important factor in the evolution of toxic gas diffusion [7], not only due to the effect of the incoming wind on the toxic gas diffusion speed, distance, and diffusion area range, but also the wind speed will change the gas diffusion mode, and then evolve into a completely different Concentration field.

1) When the wind speed of the flow field is large in the process of toxic gas diffusion, there will be an obvious "toxic gas accumulation" near the downwind to the same side wall in the confined space, and then there will be an obvious diffusion phenomenon from the side wall to the middle, with obvious turbulence effect.

2) Through the numerical simulation of the diffusion of toxic gas in the specific flow field, the distribution and evolution of the spatial concentration field under certain laws can be obtained, and the seriously polluted area and the relatively safe area can be further divided, which provides a scientific and powerful reference for emergency evacuation and decontamination.

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