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Numerical simulation of the effect of wind speed on VOCs diffusion concentration distribution in liquid cargo port area

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Abstract. The discharge of VOCs in the port area is harmful to the environment and the human body. Therefore, this paper aims at transient leakage of VOCs in cargo port area. The diffusion process was simulated with Fluent software, and this paper considered the impact of changes in wind speed on the diffusion concentration distribution. The results show that when the wind speed is higher, the earlier the initial concentration appears, the greater the concentration peak is, and the longer the VOCs spread. The increase of the wind speed is conducive to the diffusion of VOCs.

1. Introduction

At present, air pollution in China's ports is serious. The pollutants such as volatile organic compounds (VOCs) discharged by the port have spread to the periphery of the port area, seriously affecting the human health of the port area, and will spread to far areas as pollutants migrate. There are long-term effects in that area. The proliferation of pollution sources has attracted the attention of some domestic scholars.

At present, many scholars have carried out relevant researches on the issue of continuous leakage of VOCs. Zhao Chenlu et al. [1] found that the diffusion coefficient of the leakage point caused by the outside wind speed is larger than the diffusion coefficient of oil and gas molecules when there is no wind. Huang Weiqiu [2] simulated the diffusion and emission of gasoline in restricted space and found that the higher the height of the oil inlet is, the greater the oil and gas emissions. Yan Congbin [3] selected a set of CFD models for the leakage diffusion scenarios with different combinations of leak rates and wind speeds for an offshore oil and gas office module, discussed in depth the distribution and formation rules of gas concentrations, and found that the concentration distribution after gas diffusion can be in certain Time reaches steady state. However, at this stage, there is little research on the diffusion analysis of transient leakage of VOCs.

This paper aims at VOCs transient leakage accident in liquid cargo port area. Fluent software was used to simulate the diffusion process and the influence of the wind speed change on the diffusion concentration distribution was considered.

2.Model establishment

2.1 Physical Model



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This article assumes that a large number of crude oil spills from oil tanks in a liquid cargo port, resulting in the instantaneous production of a large number of VOCs gas. Considering the wide range of gas diffusion, the gas diffusion space model was selected as a large rectangular parallelepiped with a length of 350m, a width of 115m, and a height of 33m. The instantaneous leakage source was set to a length of 12.4m, a width of 6.2m, a height of 13m, and a volume of 100m3(The X-axis midpoint coordinate of the leakage source is (40,0,0)). Three monitoring points were selected within the spatial range: point 1 (100, 30, 1.6), point 2 (160, 40, 1.6), point 3 (220, 50, 1.6). The specific geometric model parameters are shown in Figure 1.



Fig. 1 Computing Domain Model

2.2Mathematical model

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2.2.1 Continuity Equation The continuity equation can be derived from the law of conservation of mass:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho u_i \right) = 0 \tag{1}$$

Where, ρ is the density of the mixture and uj is the speed in three directions (v,v,ω) .

2.2.2 Conservation of momentum equation According to the law of conservation of momentum, the momentum conservation equations in the three directions of x, y and z can be obtained. The general formula is:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_t \frac{\partial u_i}{\partial u_j} \right) + \frac{\partial}{\partial x_j} \left(\mu_t \frac{\partial u_j}{\partial u_i} \right) + (\rho - \rho_a) g_i$$
(2)

Where, μ is the effective dynamic viscosity of the fluid, μ t is the turbulent viscosity of the fluid, g is the gravitational acceleration, and P is the absolute pressure.

2.2.3 *Mass Conservation Equations* The conservation of the mass of the components can be derived from the conservation law of the component mass:

$$\frac{\partial(\rho\omega)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j \omega) = \frac{\partial}{\partial x_j} \left(\rho D_t \frac{\partial \omega}{\partial x_j} \right)$$
(3)

Where, ω is the mass fraction of the component and Dt is the turbulent diffusion coefficient of the fluid.

2.2.4 Control equation In Fluent's active control equations, the κ - ϵ mode considers both the turbulent fluctuating velocity transport and the turbulent pulsation length transport. It is a widely used turbulent model and it is more consistent with the conditions of gas leakage diffusion [4].

The control equation applied in this paper is the κ - ϵ model:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_i}{\sigma_k}\right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k$$
(4)

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e u_i) = \frac{\partial}{\partial x_i} \left[(\mu + \frac{\mu_i}{\sigma_e}) \frac{\partial e}{\partial x_j} \right] + C_{1e} + \frac{e}{k} (G_k + G_{3e}G_b) - C_{2e}\rho \frac{e^2}{k} + S_e$$
(5)

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3. Numerical simulation parameter settings

3.1 Diffusion coefficient settings

The diffusion coefficient of VOCs determines its migration and evaporation. In this paper, the diffusion coefficient of VOCs is calculated using the Fuller empirical formula [5,6]. The formula has higher calculation accuracy at the temperature of the numerical simulation of this study. Its calculation formula is:

$$D_{VA} = \frac{1.013 \times 10^{-2} \text{ T}^{1.75} (1/M_{\text{V}} + 1/M_{\text{A}})^{1/2}}{P((\Sigma V_{V})^{1/3} + (\Sigma V_{A})^{1/3})^{2}}$$
(6)

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Where, D_{VA} is the gas diffusion coefficient, m^2/s ; T is the temperature in the cargo tank, K; P is the absolute pressure of gas, Pa; M_V , M_A is the molar mass of VOCs and air, g/mol; V_V , V_A are VOCs and the molecular diffusion volume of air.

3.2 Initial Condition Settings

At the initial time, the concentration of the leakage source bleeder is set to 1 and the remaining space in the calculation domain is initialized to air. The initial setting of the overall temperature is 300K, and it is assumed that the temperature does not change during the leak. The pressure is 101325pa and the atmospheric stability is D ($-1^{\circ}C/100m$). The fluid inlet interface (ADHE surface) is set as the velocity inlet; the fluid outlet interface (BCGF surface) is set as the pressure outlet; the EFGH surface, the DCGH surface, and the ABFE surface are set as free interfaces; the ABCD surface is set as the wall surface.

3.3 Import wind speed setting

This paper assumes that the wind direction is a constant wind direction and the direction is the same as the positive direction of the X axis. The function of the inlet wind speed as a function of height [7] is as follows:

$$u_{z} = u_{1} \frac{\ln z - \ln z_{0}}{\ln z_{1} - \ln z_{0}}$$
(7)

Where, uz is the average wind speed (m/s) on the ground z height; u1 is the average wind speed (m/s) on the ground z1; z_0 is the roughness-length (cm or m), z_0 is the ground A measure of dynamic roughness, which is related to the height of roughness elements, is a function of the shape and density distribution of roughness elements [8]. The value of z_0 in this paper is 0.01m.

This paper sets up three sets of comparative numerical simulations of different wind speeds. The first group of test 10m high wind speed is set to 2.4m/s, the second group of 10m high wind speed is set to 5.0m/s, the third group of 10m high wind speed is set to 10.0m/s (after that wind speed refers to 10m high wind speed).

4. Results and Analysis

4.1 Numerical Simulation Verification

The comparison between numerical simulation results and experimental results [9] is shown in Figure 2:



Fig. 2 Comparison of simulated data and test data

It can be seen from the figure that the simulated data is in good agreement with the experimental data, but there is a deviation in the initial concentration of both. Analysis of the reasons, first of all, the deviation is due to the limitations of experimental conditions, instrumental accuracy, and other factors. Meanwhile the influence of temperature changes on the evaporation rate and saturation concentration, and the error between numerical simulation results and experimental data is ignored. Secondly, the wind direction will not change during numerical simulation. However, the wind direction may change during the actual measurement process, which causes the initial concentration to appear time error.

4.2 Effect of Wind Speed on VOCs Diffusion Concentration

The graph of diffusion concentration over time for the three monitoring points is shown in Figure 3-5.



Fig. 5 Monitoring point 3 concentration curve

Comparative analysis of Figure 4 shows two things:

(1) When the wind speed is 10m/s, the concentration of the monitoring point 1 changes at a time of 5.2s, and the concentration of the concentration detection point 1 reaches a maximum of 0.29 when the time is 7s. When the speed is 5m/s, the time is 7s. When the concentration of the monitoring point 1 changes, the maximum concentration reaches 0.21 when the time is 9.8s. When the speed is 2.4m/s, the concentration of the monitoring point 1 changes only when the time is 9.5s, and the concentration reaches the maximum when the time is 12s. This shows that with the increase of wind speed, and the advection effect of wind on the gas cloud will be intensified. the greater the wind speed is, the more obvious the transport effect is, and the concentration is higher.

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(2) When the speed is 10m/s, the concentration value is continuously detected from the 5.2s to the 19s monitoring point. When the speed is 5m/s, the change of the concentration value is continuously detected from 7s to 55s. When the speed is 2.4m/s, the change in concentration can be detected from 9.5s onwards. It can be seen that the smaller the wind speed is, the slower the diffusion of gas clouds is, and the longer the gas clouds stays.

Comparing analysis of Figure 4-6, at the same wind speed, the concentration curves of the three monitoring points (positions set by the three monitoring points, and the leakage distance from the monitoring point increase sequentially) show the initial concentration time increases with distance. The initial concentration maximum decreases with increasing distance. Under the same leak conditions, the same time, the higher the wind speed is, the earlier the initial concentration occurs. The higher the initial velocity is, the higher the initial concentration is, and the longer the velocity lasts. It can be seen from the analysis of the consequences of the accident that its danger that it is conducive to the diffusion of gas clouds When the wind speed is high, and as the diffusion progresses, the concentration rapidly decreases until it does not exist in a short period of time. This indicates that under conditions of high wind speed, the spread is fast but the damage time is short. At the same time, under a small wind speed, although the gas cloud diffusion speed is slow, the gas cloud stays for a long time, and the possibility of being ignited or causing an explosion increases. Therefore, in the case of a small wind speed, the consequences of the proliferation of VOCs are also very serious.

5. Conclusions

Based on the numerical simulation test of the leakage of VOCs in the cargo port area, the following main conclusions were obtained:

Under the influence of different wind speeds, at the same monitoring point, when the wind speed is higher, the earlier the initial concentration appears, the greater the concentration peak is, and the longer the VOCs spread. The increase of the wind speed is conducive to the diffusion of VOCs.

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