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# Numerical investigation of leaking and dispersion of carbon dioxide indoor under ventilation condition



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#### ABSTRACT

Numerical simulation of continuous release and dispersion process of carbon dioxide in a ventilated room was carried out by FLUENT with Computational Fluid Dynamic (CFD) method. The validation of the simulation method was made by comparison of simulation results with experimental data. The concentration distribution of carbon dioxide indoor was investigated. The effect of the release rate, wind speed and obstacle on gas dispersion was analyzed. Results showed that at the beginning carbon dioxide moved to the top of room by the action of jet flow. Under the condition of wind, the concentration of carbon dioxide indoor kept constant. Gas-detecting alarm device should be installed at the downwind position above the leaking hole. People should get away from the room before high concentration area forms. The concentration of carbon dioxide downwind decreased with increment of wind speed, while increased with increment of release rate. Vents or forced draft should be set to decrease the concentration appeared in windward side of the obstacle. When designing the layout of industrial workshop, it is necessary to minimize the quantity of equipment indoor or put them near the wall, away from leakage sources.

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#### 1. Introduction

With the development of modern city, chemical and petrochemical industry, confined spaces have been developed rapidly, including civil architectures, plants, underground tunnels and subways, etc. Because these buildings were relatively closed, accidents such as fire, explosion and poisoning may happen once the flammable, explosive, virulent and harmful substances release. It will cause not only wealth loss, but also casualties [1-3]. Carbon dioxide is colorless, odorless gas which is widely used in many fields of industry such as industry, food, medicine and agriculture, etc. Although carbon dioxide is non-inflammable and non-explosive, high levels of carbon dioxide in air will lead to death of people due to hypoxia and asphyxia. Currently, more research work is focused on release and diffusion of carbon dioxide outdoor [4–6], but the study on release and diffusion of carbon dioxide indoor is less [7]. Installing toxic gas alarm system is an effective safety measure for preventing the recurrence of similar accidents. But where the alarm system should be installed, and how to evacuate people in the building if such accident occurs still need further investigation.

To solve these problems, the diffusion regularity of carbon dioxide indoor needs to be studied.

In this paper, the continuous release and diffusion process of carbon dioxide indoor in a ventilated room was numerically simulated with FLUENT. The distribution of carbon dioxide in the room was investigated. The effects of release rate, wind speed and obstacle on the concentration distribution of carbon dioxide were also studied. The research results will provide theoretical basis and important reference for accident prevention and emergency rescue.

#### 2. Experiment

Carbon dioxide cylinder produced by Nanjing Special Gases Factory was used in the experiment with the volume of  $0.04 \, dm^3$  and the pressure of 10 MPa, which was  $1.32 \, m$  high,  $0.219 \, m$  in diameter. The diameter of a circular leakage hole on the top of the steel cylinder was  $0.004 \, m$ . Pure carbon dioxide leaked into the room along the vertical direction at a continuous flow rate of  $0.05 \, kg/s$ . The size of air inlet was  $0.4 \, m$  in the longitudinal direction and  $0.5 \, m$  in the vertical direction. Concentration sensors were arranged in the room (see Table 1). Firstly, the outlet pressure will be reduced to a steady value by adjusting pressure-reducing valve. The gas flow rate was obtained by adjusting the flowmeter. Then, the concentration of carbon dioxide detected by sensors will be transferred

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 Table 1

 The coordinates of four inspecting points.

	<i>x</i> (m)	<i>y</i> (m)	<i>z</i> (m)	
Sensor1	1.5	0.8	0.45	
Sensor2	1.5	0.8	0.9	
Sensor3	2.0	0.8	0.45	
Sensor4	2.0	0.8	0.9	

to computer by data acquisition system. Finally, the experimental results were obtained by data acquisition system.

The sketch of the experiment was shown in Fig. 1. The volume of the room is  $16 \text{ m}^3$ , which is 4 m in the lateral direction, 1.6 m in the longitudinal direction and 2.5 m in the vertical direction. The size of air outlet was 0.5 m in the longitudinal direction and 0.4 m in the vertical direction. The velocity of air inlet was zero in the experiment.

#### 3. Modeling strategy

#### 3.1. Basic conservation equation

The leakage and diffusion of  $CO_2$  were described by using basic equations of mass, momentum, energy and transportation equations. The solution of mathematical model was based on the equations of mass, momentum, energy and species transport conservation. Thus these differential equations used in the simulation could be expressed in the general form as follows [8,9]:

$$\frac{\partial}{\partial \tau}(\rho\phi) + \frac{\partial}{\partial x_j}(\rho u_j\phi) = \frac{\partial}{\partial x_j}\left(\Gamma\frac{\partial\phi}{\partial x_j}\right) + S \tag{1}$$

The four terms in the general equation are called time term, convection term, diffusion term and source term respectively. Where  $\tau$  is the time, s;  $\rho$  is the density of gas, kg/m<sup>3</sup>;  $\phi$  is the general variable;  $u_j$  is the velocity vector component (m/s);  $\Gamma$  is the diffusion coefficient; *S* is source term.

#### 3.2. Physical model

The physical model was shown as in Fig. 1. The three-dimensional model was  $4 \text{ m} \times 1.6 \text{ m} \times 2.5 \text{ m}$  cuboids. Wind speed was 1.5 m/s.

#### 3.3. Calculation conditions

The following assumptions were made:

- (1) Carbon dioxide released at sonic constant rate. The change of the pressure of CO<sub>2</sub> in cylinder was ignored.
- (2) There was no chemical reaction, phase change reaction and droplet deposition.
- (3) Wind direction was along the *x*-axis horizontal. Wind speed and wind direction did not change with time, location and height.
- (4) There were no apparent difference between the temperature of leaking carbon dioxide and air. So there was no heat exchange.

In this paper, the calculation domain was meshed into nonhomogeneous hexahedrons. For the wall, the standard wall function method was adopted [10].

Initial conditions: at the initial time, pure carbon dioxide was specified at the inlet. And 100% air was specified at the air inlet. 300 K was all specified at walls, fluid field, carbon dioxide and air. To choose separated solver and the implicit scheme model, the standard  $\kappa - \varepsilon$  turbulent model and component transport model were used.

#### 3.4. Validation of the calculation models

Fig. 2 shows the comparison of experimental data and simulated values of four specified points. It was found that the simulating results were in good agreement with the experimental data. It suggested that the simulation method is feasible. However some difference existed because of the error of instruments, selection of parameters and assumptions of simulation.

#### 4. Results and discussion

#### 4.1. Concentration distribution

Fig. 3 shows the concentration distribution of carbon dioxide on the plane of y = 0.8 m at 10 s, 50 s, 100 s, 150 s, 200 s and 300 s, respectively. At the beginning of the leakage, carbon dioxide moved to the top of room with a high initial momentum. Thereafter, carbon dioxide diffused along the downwind by the effect of wind, and the concentration downwind continued to increase. When carbon dioxide moved around the walls, some of them flowed from the outlet, and recirculation region formed near the wall. The concentration of carbon dioxide windward increased because of accumulation. After about 150 s, the flow field was stable and the distribution of carbon dioxide in the room was unchanged.

Fig. 4 shows the relationship between concentration of carbon dioxide and downwind distance on the plane of y = 1.0 m for different heights. The concentration of carbon dioxide was low at the bottom and high at the top of the room. The concentration stratification below leaking inlet formed obviously, while the concentration above the inlet between different heights was not stratified. After some distance from the leaking source, the concentration increased obviously with the increasing of height, and stratification appeared. Subsequently, the concentration decreased with increasing distance, and stratification disappeared. After some time, the concentration below the leaking point increased as shown in Fig. 5. However, the increment of the concentration above the leaking point was different as shown in Fig. 6. The concentration increased suddenly at the distance between about x = 1.0 m and 1.5 m which is in corresponding to the area of gas exit. The jet from the leakage had an important effect on the dispersion. Carbon dioxide diffused vertically upwards due to the high flow velocity from the leakage.

Because of the significant impacts of jet and wind, with no obvious influence by gravity, gas-detecting alarm device should be installed at the downwind position above the leaking hole. People should get to the windward area away from leaking source to escape from the accident. And people must get away from the room before high concentration area forms.

#### 4.2. Wind speed

Regarding different wind speed, the concentration of carbon dioxide with the release time at one point is shown in Fig. 7. Fig. 8 shows the change of the concentration along downwind distance when the wind speed varies. The result indicated that wind speed had strongly effect on the diffusion of carbon dioxide. The concentration of carbon dioxide downwind decreased with increment of wind speed. One reason for this was that the concentration was due to the enhancing of stratospheric transportation of gas cloud with the increment of wind speed. Moreover, as the wind speed increased, the velocity fluctuation and the turbulence intensity strengthened, and carbon dioxide rapidly dispersed correspondingly. So in order to prevent suffocation accidents, vents should be set to decrease the concentration of carbon dioxide. When the wind speed is slow, forced draft should be used.

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