Numerical Simulation for Safety Zone Evolution in Complex Flow Field under Biochemical Attack Scenarios

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Abstract. Fast construction of safety zone has been long desired in the context of chemical attack. In this paper, we propose the use of flow-field control coupled with the decontamination agent technology to minimize the harm and construct the safety zone based on computational fluid dynamics (CFD) software. Aiming at two typical environmental modes, CFD simulations provide great accuracy and more details about distribution of concentration, as well as velocity in spatiotemporal scales. Corresponding experiments are provided for validations. Results reveal the presence of coherent correlation between the airflow state and the evolution of safety zone, which is of great value for the safe design of ventilation system. We hope this work brings inspiration in chemical attack scenarios to reduce casualties.

1. Introduction
Accidental biological and chemical attacks in indoor environments can cause great damages and put serious threats on public safety. Therefore, constructing the safety zone in indoor space under biochemical attack events is highly essential.

Indoor airflow is not generally distributed uniformly and generally performs turbulent motion [1]. Variables, such as pollutants, temperature and humidity, transported by airflow motion, form the heterogeneous distribution [2]. At present, CFD software has been regarded as a powerful tool. It could provide more details on various physical quantities in spatiotemporal scales by solving numerical equations [3] and is widely applied on indoor flow field simulation [4]-[7].

Generally, pollutants are reduced or removed by means of flow field control or gas phase chemical reactions. Lim et al. performed numerical analysis of the toxic gas concentration field distribution in the indoor environment based on computational fluid dynamics. They also studied the effects of chemical reactions and turbulence on pollutant diffusion [8]. Researchers performed a quantitative analysis of the system based on the ventilation efficiency index, Net Escape Velocity (NEV). The result shows that the turbulent motion improves the pollutant discharge efficiency.

In this paper, based on computational fluid dynamics software, we propose a flow-field control couple with the decontamination agent technology to minimize the harm and construct the safety zone under different airflow environments in chemical attack. The results also reveal the presence of coherent correlation between the airflow state and evolution of the safety zone, which is of great value for the safe design of ventilation system.
2. Numerical Simulation and Experiments

2.1. Assumption
The diffusion characteristics of pollutants are affected by a diversity of factors in biochemical attacks, including indoor layouts, human interferences and external environments. To facilitate the simulation calculation, the followings basic assumptions and simplifications are supposed:
(i). The effects of human activity, lighting systems, heating systems and obstacles on the affection of poison gas are ignored;
(ii). Both air and gas are ideal gases;
(iii). There is no heat exchange with the outside world;

2.2. Basic Simulation System
In this section, we introduce the basic simulation system constructed by CFD software STAR-CCM+ [9]. The overall diagram is shown in figure 1. The system is mainly composed of an enclosed area, a release source, an air-conditioner, three windows and a decontamination device.

Figure 1. The schematic diagram of the simulation system and boundary conditions.
The size of the confined space is $10 \times 4.8 \times 3 \text{ m}$. The dimension of the source is $0.1 \times 0.1 \times 0.1 \text{ m}$ and the centroid coordinate is $(9,1,0) \text{ m}$. In this paper, the release substance is assumed as chlorine. The decontamination reactor is $0.35 \times 0.25 \times 0.4 \text{ m}$ and its position is at $(0.5,4,0) \text{ m}$ in room space. The device with 20% efficiency is used for disinfecting target gas (chlorine). Considering the cleaning effect and safety of reaction products, we choose $Na_2CO_3$ as decontamination agent. The principle of chemical reaction is
\[
Na_2CO_3 + Cl_2 = NaClO + NaCl + CO_2
\]  
(1)

There are two inlet/outlet modes considered in this work, including natural diffusion and air-conditioned mode. The boundary conditions are shown in the table 1.

| Component | Type | Boundary condition |
|-----------|------|--------------------|
| Enclosed area | temperature | 300 K |
| Release source | strength | $7 \text{ g} \cdot \text{s}^{-1}$ (constant) |
| Decontamination device | Inlet/outlet | The pressure of the inlet: $-50 \text{ Pa}$; The velocity of the outlet: 5 m/s. |
| Inlet/Outlet mode | Natural diffusion | Windows and the air-conditioner are all closed. |
| | Air-conditioned mode | All the windows are closed and the air-conditioner is open. The pressure of the air-conditioner inlet: -3.5 Pa; The velocity of the air-conditioner outlet: 6 m/s; |
2.3. Physical Model

The physical models in CFD simulation contain the Standard k-ε Turbulence Model, Eddy Breakup (EBU) and the Reactive Fluid Model. The Standard k-ε Turbulence Model is a typical two-equation model, which is first proposed by Spalding and Launder in 1972 [10]. Transport equations for $k$ and $\varepsilon$ are defined as:

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

(2)

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_i} \right] + C_{1e} \frac{\varepsilon}{K} (G_k + C_{3e} G_b) - C_{2e} \rho \frac{\varepsilon^2}{K} + S_\varepsilon,$$

(3)

where $G_k$ and $G_b$ are the production terms of the kinetic energy $k$ caused by the average velocity gradient and buoyancy, respectively. $C_{1e}, C_{2e}$ and $C_{3e}$ are the empirical constants. $Y_M$ is the expansion parameter in the compressible turbulence. $\sigma_k$ and $\sigma_\varepsilon$ are the Prandtl numbers corresponding to the kinetic energy $k$ and the dissipation rate $\varepsilon$. $S_k$ and $S_\varepsilon$ are source items.

At the same time, the EBU model is assumed that the average rate of chemical reaction is independent of chemical dynamics, and only depends on the turbulent mixing between the reactants. The high $y^+$ wall treatment in the Standard k-ε model modeling the flow in the near wall area.

2.4. Validation

In this section, we present mass transportation experiments under specific conditions for validating the correctness and reliability of the CFD simulation models. Ethanol is seemed as the toxic source. A vertical fan is arranged in the conference room for airflow disturbance creation. A concentration sensor is used to collect signals every 3 seconds in 5 minutes. The correlation coefficient ($R$) is used to quantify the quality of the coherence. The definition of $R$ between $Y$ and $\tilde{Y}$ reads:

$$R = \frac{\text{Cov}(\tilde{Y}, Y)}{\sigma_{\tilde{Y}} \sigma_Y},$$

(4)

where Cov represents covariance factor and $\sigma_{\tilde{Y}}, \sigma_Y$ represent the standard deviations. As shown in figure 2, the probing concentration in a specific position, namely, $C$, is divided by the maximum concentration $C_{\text{max}}$ over time. The figure shows the correlation between experiment results and CFD calculations. The results that $R$ is larger than 0.911 in different modes of the fluid fields, suggest an acceptable consistency between the numerical simulation and experimental measurement results.

![Figure 2](image.png)

Figure 2. Comparisons of concentration ratio in different modes in experiments and CFD simulations. (a) natural diffusion mode; (b) air-conditioned mode.

3. Results and Discussion

In this section, we mainly verify the effect of the decontamination in two environmental modes and analyse the relationship between the evolution of the safety zone and the distribution of flow field. The area, with concentration lower than 0.0189 ppm [11], [12], is defined as the safety zone. We select $z = 0.8$ m as the observation plane.
3.1. Natural Diffusion

In the natural diffusion mode, the strong airflow of the decontamination reactor outlet generates two eddy currents in opposite direction are generated rapidly at the beginning. Poisonous substances diffuse following the airflow of the Vortex 2, and the eddy promote the toxic substances propagation. Therefore, the volume of the safety zone is further narrowing. At the same time, the force of Vortex1 and chemical decontamination together hinder the further diffusion of toxic substances and the hazard substances near the reactor inlet is cleaned through adsorption. The flow filed distribution is shown in figure 3. The concentration field evolution is shown in figure 4.

![Figure 3](image1.png)

**Figure 3.** Velocity field distribution at T=20 s and T=60 s in the natural diffusion environment. The left column is graphic display mode and the right column is line integral convolution display mode.

![Figure 4](image2.png)

**Figure 4.** Concentration distribution evolution of toxic gas in the natural diffusion mode.

3.2. Air-conditioned Mode

In the air-conditioned mode, the indoor airflow is messier. Figure 5 shows the velocity field distribution at a steady state. The three eddy currents are created because of the airstream encounter...
from the decontamination device outlet and the air-conditioning outlet separately. The rotating directions of the Vortex 1 and the Vortex 2 are opposite. While the toxic substances move with the airflow, the reverse flow of the Vortex 1 hinders the diffusion of toxic substances and removes pollutants under the action of the decontaminating material, and forms a safety zone. Figure 6 present the evolution of safety zone from the beginning to stability.

**Figure 5.** Velocity field distribution at T=30s in air-conditioned mode. The left is graphic display mode and the right is line integral convolution display mode.

**Figure 6.** Concentration distribution evolution of toxic gas in air-conditioned mode.

4. **Conclusion**

This manuscript elaborates the construction and evolution of the safety zone in the indoor biochemical attack events based on the CFD technology. Aiming at two different environmental modes, we build numerical simulation models to calculate the distribution of concentration field and velocity field. Experiments validation are also provided. Results show effectiveness of safety zone construction and reveal the high correlation between the distribution of safe area and turbulent flow. In the meanwhile, the vortex generated by outlet airstream may accelerate the hazards diffusion. Therefore, the correct flow field control and decontamination material coupling are essential to enlarge range of safety zone.

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