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Pressured liquid chlorine leakage accident simulation in highway tunnel

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Abstract
With the national economic development, China's transportation infrastructure has also made great progress, particularly in the highway. How to reduce the accident consequence that occurred in the highway tunnel has been the tropical topic in China. The liquid Chlorine accidental leakage in highway tunnel was exemplified for the poisonous gas dispersion consequence analysis using computational fluid dynamics. First, the GAMBIT code was used to create geometrical models and generate meshes. Second, by using the FLUENT code, the Chlorine gas dispersion in the highway tunnel was simulated and the scenarios with different leak sources were discussed. Case study shows that the FLUENT code was useful on the simulation of gas dispersion in highway tunnel that serves the prerequisite for the further research.

Keywords: Highway tunnel, FLUENT code, Poisonous gas, Consequence analysis.

1. Introduction
October 24, 2001, in Swiss, the Alps Gotthard road tunnel with its total length of 16,900 m, two trucks collided head-on and resulted in the conflagration. The fire in the tunnel burned day and night, which caused 11 casualties, 40 cars burned. Part of the casualties was killed by the smoke produced by the burning tires under bad ventilation conditions.
As China's industrial development and substantial growth in the transportation of dangerous goods, toxic chemicals transportation was highlighted the safety problems gradually. In order to improve driving conditions and transportation efficiency, the highway tunnel was built to cross the river and mountains and facilitate the transportation efficiency. According to incomplete statistics, the number of tunnels so far has surpassed 1100 in China, the size of tunnels also increased accordingly. Consequently, traffic flow and vehicle speeds surged that resulted in the higher probabilities of the accidents occurred in highway tunnel.
Although the probability of toxic gas leakage occurred in the tunnel is very low, space inside the tunnel was limited and relatively confined, vehicles and passengers were difficult to evacuate in case of accidents, which caused tremendous loss of lives and properties [1, 2].
The former study on diffusion of hazardous gas leakage focused mainly on the industry accidents in the workshop. The mathematical models were established and applied mainly to dispersion without obstruction. However, when it applied to narrow space inside the tunnels, these dispersion models needed to be further validated under specific spatial structure. So, this paper adopted the methodology of

computational fluid dynamics (CFD) and the classic CFD code - FLUENT as the tool to simulate the dispersion of the toxic gas leakage inside the tunnel. In case study, the characteristics and impact factors of the dispersion in the tunnel were took into consideration in detail.

2. The description of basic models and software

In terms of the model complexity, dispersion models can be divided into three categories: experience model; applied model; and research model.

The experience model and applied model have been used for a long time in engineering application. Both of them were designed under different basic assumptions, so the two were characterized by the quick calculation, good operability, and high conveniences together with certain errors in the results. Further, it can not present the details of diffusion and apply to complex terrain with obstacles.

Judging from the research background, this paper focused on the simulation of toxic gases diffusion in the tunnel in confined space with a lot of obstacles. In order to obtain and analyze the detailed progress of diffusion, the research model based on the computational fluid dynamics was more suitable to be the tool. Research model described the process of the diffusion controlled by the basic conservation equation including quality, momentum, energy and component equations, etc. Combined with initial and boundary conditions, it can put forward the fine description of gas dispersion.

FLUENT code was widely used in the study of urban atmospheric environment and the proliferation of pollutants, and the simulation results match the wind tunnel experiments well.

Li Lei used FLUENT code to study the flow field and proliferation of pollutants in metropolitan, established a three-dimensional model for the road cross, and discussed the concentration of pollutants affected by the layout of constructions and wind direction [3].

Cheng-Hsin Chang also used FLUENT code to study the transfer of pollutants in the city's downtown and put forward the entire simulation process. Also when the numerical simulation results were compared with experimental data, he found out the concentration field of the pollutants had little differences with that of the wind-tunnel experiment [4].

All of the above showed that FLUENT code can be used to study the proliferation of toxic gas dispersion in complex terrain.

3. Model used and mesh generation

All of the CFD, in one form or another, was based on the fundamental governing equations of fluid dynamics-the continuity, momentum, and energy equations. Except for the chemical reaction in the process of diffusion, the governing equations under Cartesian coordinate system drived three-dimensional steady in-viscid flow can be summarized as follows [5,6].

$$\frac{\partial}{\partial t}\iiint_V Q dV + \iint_{\partial V} F \cdot n dS = 0 \tag{1}$$

where,

$Q = (\rho, \rho u, \rho v, \rho w, \rho e)^T$: Conserved vectors;

$\rho, (u, v, w), e$: Density, velocity, and energy;

∂V : The boundary of the fixed zone V;

n : Exterior Normal-vector;

F : Flux-Vector that includes convection and viscosity flux-vector, $F = F_c - F_v$ [7];

F_c, F_v were given below:

$$F_c = \begin{bmatrix} \rho ui + \rho vj + \rho wk \\ (\rho u^2 + p)i + \rho uvj + \rho uwk \\ \rho uvi + (\rho v^2 + p)j + \rho vwk \\ \rho uwi + \rho vwj + (\rho w^2 + p)k \\ (\rho ue + up)i + (\rho ve + vp)j + (\rho we + wp)k \end{bmatrix}, \quad F_v = \begin{bmatrix} 0 \\ \tau_{xx} i + \tau_{xy} j + \tau_{xz} k \\ \tau_{yx} i + \tau_{yy} j + \tau_{yz} k \\ \tau_{zx} i + \tau_{zy} j + \tau_{zz} k \\ \prod_x i + \prod_y j + \prod_z k \end{bmatrix} \tag{2}$$

where,

$$\begin{aligned} \prod_x &= \tau_{xx} u + \tau_{xy} v + \tau_{xz} w - q_x \\ \prod_y &= \tau_{yx} u + \tau_{yy} v + \tau_{yz} w - q_y \\ \prod_x &= \tau_{zx} u + \tau_{zy} v + \tau_{zz} w - q_z \end{aligned} \tag{3}$$

Viscous strain can be summarized by,

$$\begin{aligned} \tau_{xx} &= 2\mu u_x - \frac{2}{3}\mu(u_x + v_y + w_z) \\ \tau_{yy} &= 2\mu u_y - \frac{2}{3}\mu(u_x + v_y + w_z) \\ \tau_{zz} &= 2\mu u_z - \frac{2}{3}\mu(u_x + v_y + w_z) \\ \tau_{xy} &= \tau_{yx} = \mu(u_y + v_x) \\ \tau_{xz} &= \tau_{zx} = \mu(u_z + w_x) \\ \tau_{yz} &= \tau_{zy} = \mu(v_z + w_y) \end{aligned} \tag{4}$$

The proliferation controlled by the *FICK* law originated in the concentration of uneven that can be quantified by the concentration gradient q.

$$q_x = -k\frac{\partial C}{\partial x}, q_y = -k\frac{\partial C}{\partial y}, q_z = -k\frac{\partial C}{\partial z} \tag{5}$$

The transport equations of turbulent energy k and dissipation ratio ε also were included in the equation series.

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j \frac{\partial k}{\partial x_j} - \left(\mu + \frac{\mu_\tau}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] = \tau_{tij} S_{ij} - \rho\varepsilon + \phi_k \tag{6}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho u_j \varepsilon - \left(\mu + \frac{\mu_\tau}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] = C_{\varepsilon_1}\frac{\varepsilon}{k}\tau_{tij} S_{ij} - C_{\varepsilon_2} f_2 \rho \frac{\varepsilon^2}{k} + \phi_\varepsilon \tag{7}$$

The governing equations associated with some auxiliary equations (equation of state, heat formula, etc.) can make equations closed, together with the set of conditions (initial and boundary conditions), which eventually constituted a complete mathematical problem.

FLUENT code contained quality, momentum, and energy and composition equation of fluid. Users will select and configure them under specific circumstances. For the case of turbulence, FLUENT provided wide range choices of models, such as the *Spalart-Allmaras* model, *K-ε* model, *K-ω* model and Reynolds stress model etc. As for the special needs of case study, *K-ε* standard model can get better results and be chosen to calculate the turbulence effects here [8].

In this paper, the targeted tunnel section was chosen from part of *TanYugou* tunnel of *Badaling* expressway in Beijing. *TanYugou* tunnel was three-lane one-way tunnel whose total length was 3455 m. It was the largest large-span road tunnel in China and also in Asia. In order to construct the model easily, we simplified the lower part as rectangular and top as arch [9]. As shown in Figure 1.

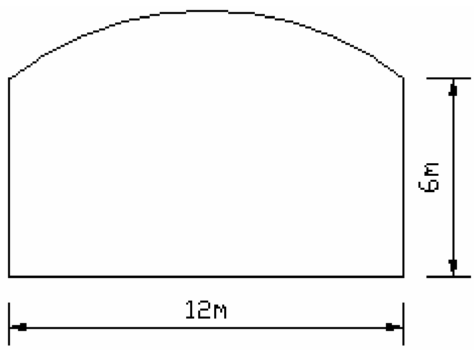

Figure 1. The cross-sectional profile of tunnel

The accident scenario was defined as liquid Chlorine leakage in a tanker passing by the tunnel. The physical boundary was confined to be a section of 100 m down wind in proximity of the leak source. The leak source was a hole with diameter of 10 cm; the leakage rate was 0.5 kg/s. Collision caused traffic jams inside the tunnel with vehicle spacing of 4 m.
In order to construct the geometric model easily, it assumed that there were only two types of vehicles in the tunnel. Furthermore, it also assumed that the crane was 13 × 2.5 × 3 m (L × W × H), 0.6 m from the ground; the car was 4 × 2 × 1.5 m (L × W × H), 0.3 m from the ground. Completed construction of physical boundary using Gambit code was shown in Figure 2.

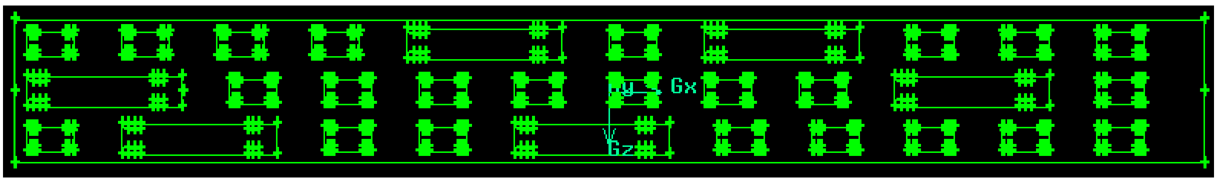

Figure 2a. The vertical view of tunnel geometric model

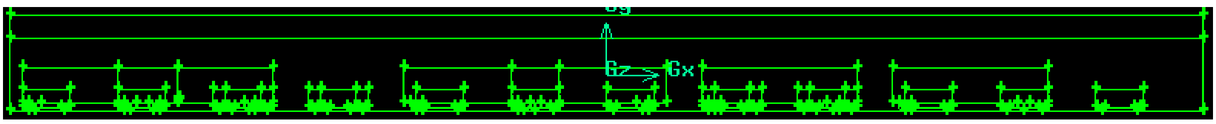

Figure 2b. The side view of tunnel geometric model

After the physical boundary was set up, Gambit code adopted unstructured grid to mesh the geometric model and all of the grids were quadrilateral. After the completion of meshing, the grid file was input into the FLUENT code.

4. The analysis on the simulation results

4.1 The analysis of the wind field in tunnels

Figure 3 showed the velocity vector contour with the wind speed 1.5 m/s.
Case study showed the wind speed in the gap before and after vehicles was smaller than its adjacent space obviously, and the vortexes were produced in some regions. These results matched other similar numerical simulations and experimental observations well [10].
From Figure 3a, it can be found out that the wind speed was gradually increased across the upper space because of poor ventilation conditions in the lower part of the tunnel. When the amount of wind

circulation remained unchanged, the wind speed increased in the higher part where no obstructions existed.
From Figure 3b, the largest local wind speed emerged on both sides of vehicles at the entrance of the tunnel. And more far away from the wind inlet, smaller the wind speed was. It was mainly due to frictions between vehicles and the wall.

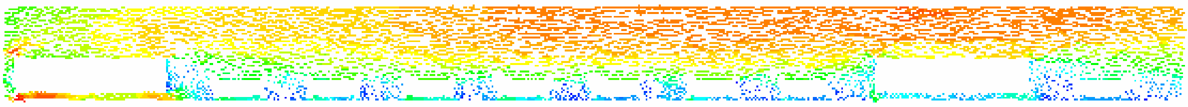

Figure 3a. The wind field contour of the central longitudinal profile
Notes: Red indicates the greatest speed; Blue indicates the minimum speed

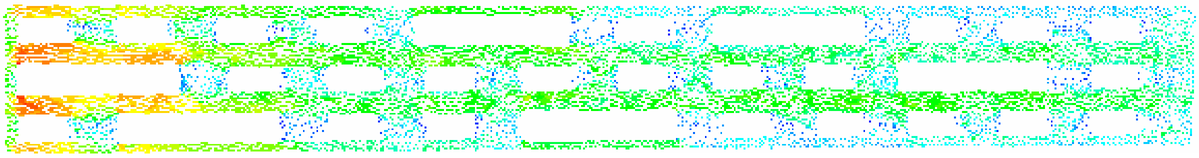

Figure 3b. The wind field contour in profile 1.5m from the ground
Notes: Red indicates the greatest speed; Blue indicates the minimum speed

4.2 Consequence analysis of Chlorine leakage
In this paper, we assumed that the Chlorine leakage accident caused traffic jams in the tunnel. And we also assumed that the leakage rate was 0.5 kg/s, the wind speed 1.5 m/s and the leak source 1 m from the horizontal ground.
From Figure 3, it can be seen that the distance of Chlorine proliferation in the upper part of the tunnel significantly higher than that of near the ground. This was because the upper part of the tunnel without obstruction was conducive to the ventilation, Chlorine proliferation in the top under higher wind speed was faster than that of the lower, and then reached the top after 10s. Also it can be seen that the Chlorine concentration in the gap before and after the vehicles was smaller than that of the surrounding space. The main reason was the relatively lower wind speed and vortex formation, which made the Chlorine outside be difficult to access to these regions in accordance with relatively slower progress. Here, the Chlorine concentration contour was consistent well with the wind field acquired before.
Figure 4 illustrated the Chlorine concentration distribution at the central longitudinal profile after leakage occurred 20s and 40s later. Apart from these, FLUENT code can also obtain Chlorine diffusion contour of different other profiles. Figure 5 showed the contour after 20s and 40s in the profile 1.5 m from the ground.
In the horizontal surface 1.5 m from the ground, as wind speed in the gap between the lanes was larger, the wind speeds around both sides of the walls rapidly decreased for the obstacles and frictions which resulted in the slowdown of Chlorine proliferation in the crosswind profile. It can also be seen from Figure 5, after 40s, Chlorine was still not fill with the whole plane.

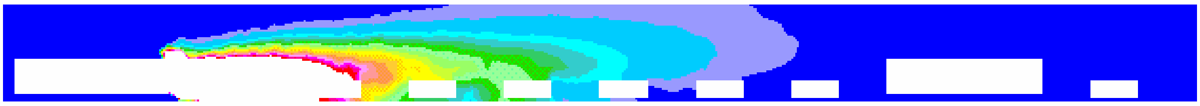

Figure 4a. The Chlorine concentration contour of the central longitudinal profile (20s)

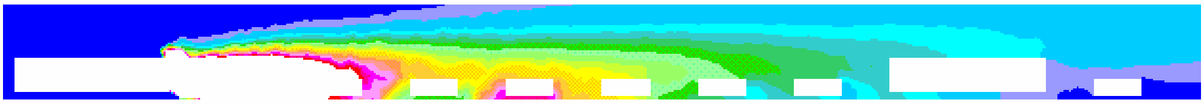

Figure 4b. The Chlorine concentration contour of the central longitudinal profile (40s)

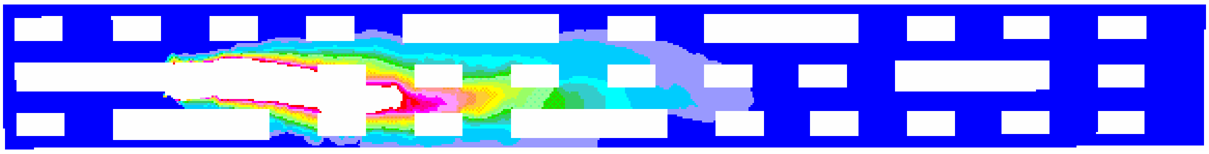

Figure 5a. The Chlorine concentration contour in profile 1.5 m from the ground (20s)

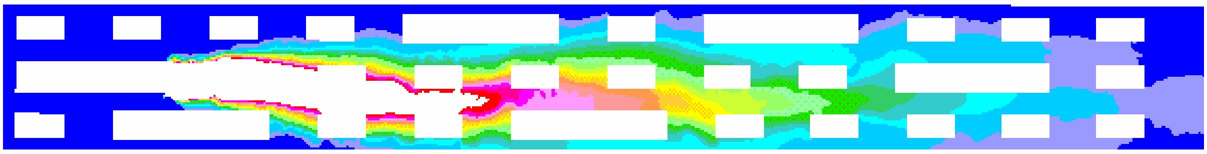

Figure 5b. The Chlorine concentration contour in profile 1.5 m from the ground (40s)

4.3 Impacts from the variation of leak source

Case study reassumed that leak source was turn upward at the top of tankers. Other initial and boundary conditions remained unchanged.

Figure 6 showed Chlorine concentration contour of the central longitudinal profile after 20s and 40s. It can be seen from Figure 6 that the leaked Chlorine quickly reached the top, and expanded downwind along the upper part. Chlorine concentration at the lower part of the tunnel between vehicles was greatly less than that of upper part in the same longitudinal profile. In conclusion, the higher the leak source is, the more mass fractions of Chlorine are.

Compared to the leak source 1m high at the rear, the Chlorine concentration should be much smaller than that of 1.5 m from the ground. As shown in Figure 7, also in this profile it was not the nearer from the leak source, the greater the Chlorine concentration was, but hump-shape distribution. The main reason was Chlorine's density was much greater than that of air that dropped down to the group by gravity, so there will be a high concentration zone at a certain distance from the leak source.

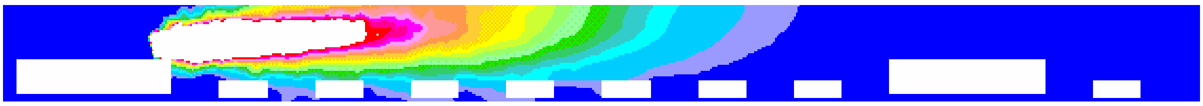

Figure 6a. The Chlorine concentration contour of the central longitudinal profile (20s)

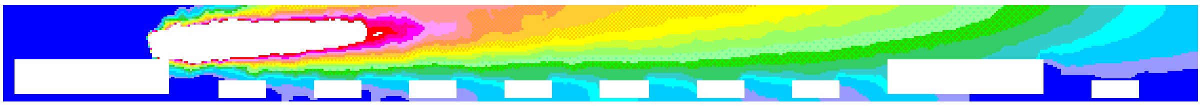

Figure 6b. The Chlorine concentration contour of the central longitudinal profile (40s)

Figure 7a. The Chlorine concentration contour in profile 1.5 m from the ground (20s)

Figure 7b. The Chlorine concentration contour in profile 1.5 m from the ground (40s)

5. Conclusions

In this paper, FLUENT code was used to simulate the dispersion of liquid Chlorine tankers leakage accident in TanYugou tunnel. According to the actual size of TanYugou tunnel and vehicles passing by, we established a simplified scenario in which typical accident was analyzed. And then the differences among different accident scenarios were discussed under different leak sources at different altitudes.

Although the simulation results match theoretical analysis well as to the simplified accident scenarios, further validation based on experimental data is needed. The next step is to reproduce the scenario under laboratory circumstances, and then the calculation accuracy can be authenticated by wind tunnel experiments. On the other hand, only the Chlorine concentration is calculated here. It can be further transformed into the dangerous zone considering the acute poisoning dose, which provides the basis for the emergency rescue and supports the performance-based tunnel design in order to reduce the harm when the toxic gas leaked.

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