GAS AGENT RELEASE SIMULATIONS USING CFD

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***Abstract*– The answer to chemical and biological attacks relies on the ability to monitor and detect the presence of an agent. The aim of this study is to verify the efficacy of a subway smoke extraction system that contains a toxic gas contamination area. A Brazilian subway station located in Rio de Janeiro was selected as a model scenario. Three case studies were examined that activated the SES in exhaustion and ventilation modes. The visualization of the velocity fields and toxic gas concentration profiles showed that when the SES was activated in the extraction mode, it took a few minutes for all of the gas to be taken into the galleries. When the SES was activated in the ventilation mode, the contaminated air was directly disposed into the atmosphere. Therefore, our results show that CFD can be used to propose a contingency plan using the subways' ventilation equipment.**

***Keywords*– CFD, dispersion, chemical defense.**

I. INTRODUCTION

The new world order has enlarged the political, economic and military powers of the hegemonic nations. In addition, strong nationalisms and fundamentalisms have been rising, resulting in international terrorist actions around the world, such as suicide attacks using airplanes in New York and Washington and bomb explosions in Madrid and London. These events reveal that the national defense question is not only the concern of specialized groups, but is becoming a relevant matter to all citizens. Therefore, the scientific community must consider the security of the civilian population and work to find solutions to terrorist attacks.

In particular, the answer to chemical and biological attacks requires the ability to monitor and detect the presence of agents (Fitch *et al*., 2003), to restrict the affected area and to identify the people exposed to the agent. This must be done prior to the decontamination of people, equipment and construction.

In fact, new and sophisticated techniques of chemical and biological defense (CB) have been developed (Shenoi, 2003; Bhalla and Warheit, 2004). The sensitivity, automation and reliability of detection systems and agent identification methods have improved. Several dispersion models and simulations of chemical warfare have been carried out (Scorpio *et al*., 2003), which has facilitated the process of sensor positioning, in addition to other improvements.

Computational fluid dynamics (CFD) is a powerful tool that can be used to simulate chemical and biological attacks, which can occur in a variety of situations ranging from indoor scenarios (Fitch *et al*., 2003; Zhao *et al*., 2004) to attacks on continents. Indoor environmental studies investigate heating, ventilation, and air conditioning (HVAC) issues and do not demand massive computation.

There are some studies that the validation is not possible. They are just the defense and hazardous studies. It can be cited Kukkonen *et al*. (2001), Scorpio *et al*. (2003) and Zhao *et al*. (2004). In the first article, the atmospheric dispersion of Sarin was carried out. In the second, the authors studied the release of a bio-agent in a room. And in the third, the authors determined a ventilation strategy to defend indoor environment against contamination by a contaminant source.

The aim of this work is to use CFD tools to simulate a toxic gas release event in a Brazilian subway station located in Afonso Pena's station in Rio de Janeiro. To reach this objective, the simulation work was divided into three main parts: *i*) establish subway station geometries and boundary conditions; *ii*) choose a satisfactory turbulence model to model the airflow; and *iii*) choose an optimal grid for the finite volume algorithm. For the first part, the data on the station's geometry were collected *in loco* in addition to the information on the ventilation/exhaustion systems located in the adjacent train tunnels. In order to select satisfactory fluid dynamics conditions, experiments were conducted using LVEL and κ-ε turbulence models. The chosen grid was structured and non-uniform so it would be possible to compute the more detailed fields near the release area and around obstacles. Finally, the analysis of the resulting data was made by visualizing the velocity fields and the toxic gas concentration profiles. The present study is a CFD simulation and further experimental analysis should be performed.

II. FUNDAMETALS

A. Contingency Plan

A terrorist attack can be treated like a disaster event, thus one may assume that the procedures used to deal with both types of situations are similar. Risk analysis indicates that a contingency plan should be composed of four phases: notification, first-response, characterization and restoration (decontamination and remediation) (Fitch *et al*., 2003; Raber *et al*., 2002).

The first necessary condition prior to forming a decision-making framework is the ability to detect a chemical or biological agent. After that, notification is possible. The first-response phase is composed of emergency actions that public health departments must carry out. Finally, the characterization and restoration phases include dispersion modeling and simulation of warfare contamination agents. This can include flow fields and

concentration distributions obtained using CFD tools. CFD simulations are virtual experiments that can reveal relevant information such as the duration and extent of decontamination, sensor positioning and ventilation strategy (Zhao *et al*., 2004).

B. CFD

Complex problems that involve transport phenomena can be treated with CFD. Profiles of physical properties such as velocity, pressure, temperature, density and mass fraction can be computed. This approach allows for an accurate prediction of all of these properties when it is not possible to carry out the experiments, for instance during a terrorist attack.

In this work, we employed the computer program **PHOENICS** (**P**arabolic, **H**yperbolic **O**r **E**lliptic **N**umerical **I**ntegration **C**ode **S**eries). This program simulates phenomena involving single and multi-phase fluxes, mass and heat transfer, as well as chemical reactions. The program solves the mass, momentum and energy conservation equations in finite domains in both the stationary and transient states and in one-, two- and three-dimensional geometries (Polis, 2010).

C. The transport phenomena equations

For compressive, non-steady flow, the equations for continuity, momentum conservation and chemical concentration can be expressed in the general conservation form in rectangular coordinates (Patankar, 1981):

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x}(\rho u\phi)+\frac{\partial}{\partial y}(\rho v\phi)+\frac{\partial}{\partial z}(\rho w\phi)= \frac{\partial}{\partial x}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma^{\phi}\frac{\partial\phi}{\partial z}\right)+S^{\phi} \quad (1)$$

where ϕ is a generic variable that depends on the transport phenomena under question, ρ is the density, u, v and w are the components of the velocity fields in the x, y and z directions, respectively, Γ^{ϕ} represents the effective exchange coefficient of ϕ and S^{ϕ} is the source rate per unit volume.

D. Turbulence Models

The Reynolds-averaged Navier-Stokes (RANS) turbulence models can be separated into three main categories, namely, algebraic (zero-equation), one-equation and two-equation models (Wilcox, 1993). This classification is based on the number of differential equations used by the corresponding turbulence model. The algebraic models are mixing-length models that use the Boussinesq eddy-viscosity approximation to compute the Reynolds stress tensor. There are not differential equations in these models so they are not computer intensive. However, the calculation of the mixing-length is strongly related to the physical situation.

For the one-equation models, the turbulence length scale is associated with some typical flow dimension. These models are not popular because they are incomplete, that is, additional information about the flow must be known, other than the initial and boundary conditions. Two-equation models, on the other hand, do not require any prior knowledge of the turbulence structure,

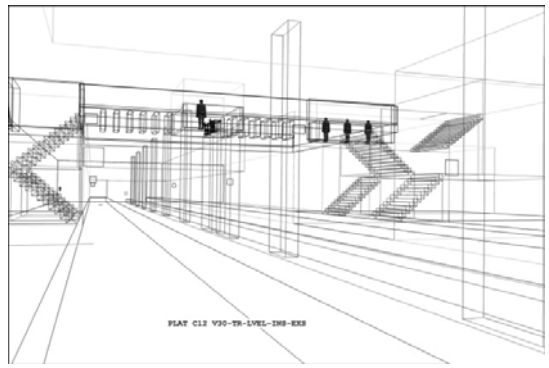

Figure 1. View of station's wireframe

and they calculate the turbulence energy κ and the dissipation rate ε (κ- ε models) or the specific dissipation rate ω (κ- ω models).

The LVEL model is a zero-equation model that is useful for engineering applications employing simple geometries. LVEL is an acronym composed of L, the distance from the nearest wall, and VEL, the local velocity.

The κ-ε models are the most popular turbulence models. They are based on the concept of eddy viscosity and utilize two differential equations, which are connected to the turbulence energy and the dissipation rate. The idea behind these models is to relate the rate of production of turbulent energy by Reynolds stresses to the rate of viscous dissipation.

III. METHODS

A. Case Description

In order to run a realistic simulation and to allow for the possibility of future experimental validation, a Rio de Janeiro subway station was selected the Afonso Pena subway station. This station has two platforms (A and B), with a mezzanine that is connected to the platforms by two large sets of stairs. The ticket offices, the turnstiles, the supervisor's room and several other staff rooms are located on the mezzanine. These rooms are usually locked and thus, in this study, they were considered to be solid blocks. The entrance stairs to the subway station are also on the mezzanine. Figure 1 shows the subway station geometry.

One of the reasons for selecting the Afonso Pena station is the simplicity of its ventilation system. Unlike other subway stations that have complex central ventilation systems, this station has only eight wall fans. These 0.65m diameter fans are distributed throughout the station, four fans for each platform, and the air flow rate is about 18 m^3/s.

Another piece of equipment that influences the ventilation in the station is the **S**moke **E**xtraction **S**ystem (SES). There is at least one SES located in each section of the train tunnel, although there may be more than one in the same section of the station, especially in the larger stations. The SESs are equipped with two or three 2.5 m diameter industrial fans, with an air flow capacity of up to 50 m^3/s, which leads to air velocities of 0.86 m/s in the tunnel. The fans work by blowing atmos-

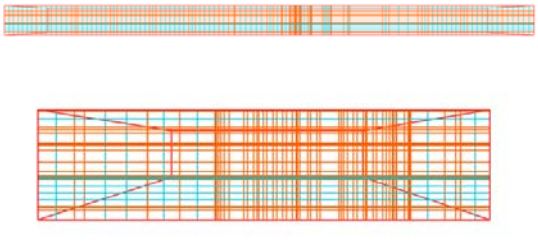

Figure 2: The mesh used for case study 2 and the zoom on the mezzanine

pheric air into the tunnel or blowing the tunnel air out into atmosphere. The supervisor, when informed of any incident in the station, may combine the two methods of operation in order to speed up smoke extraction.

The three case studies were set up to investigate the efficiency of the subway smoke extraction equipment under different conditions and how well a system designed to disperse smoke could disperse a chemical contaminant. The analysis was based on the following scenario. First, a steady sate velocity field, which is generated by the small fans, was obtained. Afterwards, chlorine gas was dispersed. Finally, the SES was turned on in order to develop an exhaustion or ventilation condition. We discuss the methodology of each case study in the following sections.

B. Case Study 01

The steady state velocity field was established when the SES was activated. The domain size adopted was 119.2 m x 20.25 m x 10.43 m. Two lengths of 50 m were added to the geometric representation to aid in analysis of the velocity profiles. Two non-uniform cartesian grids (x,y,z directions) of 100 x 50 x 22 and 200 x 50 x 22 were used, and the mesh convergence can be observed on calculated variables. The κ-ε turbulence model was employed.

C. Case Study 02

A scenario of contaminant gas leakage on platform A was investigated. The domain size adopted was 166 m x 37.10 m x 9 m, and it was initially filled with air at 20ºC. The length of the station is 146 m and two lengths of 10 m were added to allow the bulk velocities. The reported results were obtained using a non-uniform cartesian grid of 140 cells in the x-direction, 70 cells in the y-direction and 29 cells in the z-direction (284,200 total cells), see Figure 2. Similar results were also obtained using a fine cartesian mesh with 200 x 50 x 22 cells; therefore, the convergence mesh was allowed. In order to understand the dispersion phenomenon and to test the efficiency of SES for extracting the contaminant, the transient phenomenon was studied. The total simulated time was 240 seconds; the employed scheme of time dependency and the boundary conditions are illustrated in Table 1. The simulations were conducted using the LVEL turbulence model and κ-ε model.

To assure that the solutions will converge, the PHOENICS convergence wizard (CONWIZ) was used whenever the data were sufficient and self consistent.

Table 1: Boundary conditions and event definition

Time (s)	*Condition*	*Time steps*
0-5	Steady state, wall fans powered on, SES powered off	2
5-10	Leakage of 0.055 m^3/s of contaminant in the position (62.00, 1.36, 1.00)	20
10-20	Diffusion and advection of contaminant	40
20-64	Idem	27
65	SES powered on with velocity u = -0.86 m/s	1
66-180	Extraction of contaminant to the tunnel	74
180-240	Idem	12

Among other features, it chooses 'initial guesses', relaxation factors, upper and lower limits of variables, increment limits, and other convergence-promoting devices (Polis, 2010).

D. Case Study 03

A continuous contaminant gas leak on the mezzanine was created. The continuous leakage simulation was considered to be action by a persistent agent, which is the ability to evaporate in more than 24 h (Shenoi, 2002). Although chlorine is not generally a persistent agent, we were able to consider it one in this case because gas was flowing throughout the simulation. The PHOENICS convergence wizard (CONWIZ) was used here as well.

E. Monitoring and Convergence

The values of the variables in all cases were monitored at seventeen different points spread over the platform, and the goal of these measurements was to verify the results obtained from the different simulations. These monitoring points were located at a height of 1.70 m, which is the estimated height at which people breathe.

The case studies involve chlorine, which is a gas at atmospheric pressure and room temperature. It is a respiratory irritant, and may lead to death. The detection limit by the human nose is about 0.2 ppm and a lethal dose based on the LD_{50} (the concentration required to kill half the members of a tested population) is 19 $g.min/m^3$ (a mole fraction of approximately 6.62 10^{-3} at 1 atm and 298 K). The iso-concentration surfaces of the contaminant were monitored. The concentration was assumed to be safe for people at a mole fraction of 6.6 10^{-4}. This value represents one tenth of the mole fraction of chlorine gas at the LD_{50} at atmospheric pressure and 298 K, and so it is sufficient to assume that this is safe for human exposure.

III. RESULTS AND DISCUSSION

The velocity fields, contaminant iso-concentration surfaces and velocity profiles were computed over time for the monitoring points for the three case studies. Figure 3 depicts the steady state velocity field of case study 01, the preliminary simulation. The velocity reached the value of 11 m/s inside the diffuser, which is consistent with the value of the theoretical flow, 9.82 m/s. As may be observed in Fig. 3, the velocity field is plug flow distributed in the tunnels. Due to the asymmetry in the ge-

ometry, there is a difference between value of the velocity before and after the diffuser. It can also be seen that the flow is fully developed after 20 m, i.e. the plug flow is well established. This simulation took 15 hours in a Pentium IV 3.2 Ghz (1 Gb RAM), the same computer used for the other simulations in this work.

In the second case study, the contaminant was released over a 5-10 s time interval. The first-response time achieved by the subway station staff was one minute. This is a low estimation of the first-response time, considering the lack of automatic sensors for chemical agents and thus that the detection of a contaminant at this location probably occurs symptomatically. This may seem unrealistic, but one of the aims of this study is to show how a quick first response time is vital to the success of a counterterrorism action.

After 60 s, the SES was activated. The simulation ran for 240 s, almost 3 min after the SES activation. Some representative results are given in the following figures. In Fig. 4, the air velocity vector field at the x-z cross-section is given for Platform A, the platform where contaminant release occurred, after the activation of the smoke extraction system.

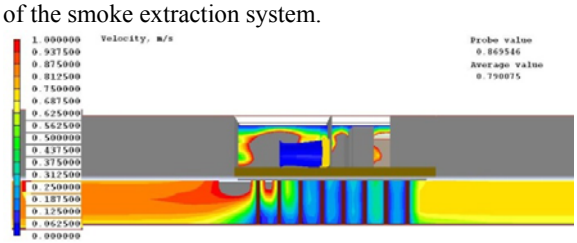

Figure 3: Air velocity field at the x-z cross section and next to diffuser.

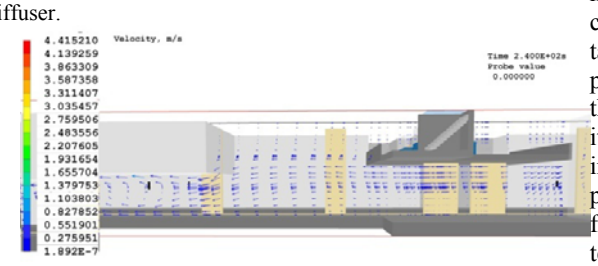

Figure 4: Air velocity field at the x-z cross section after activation of SES.

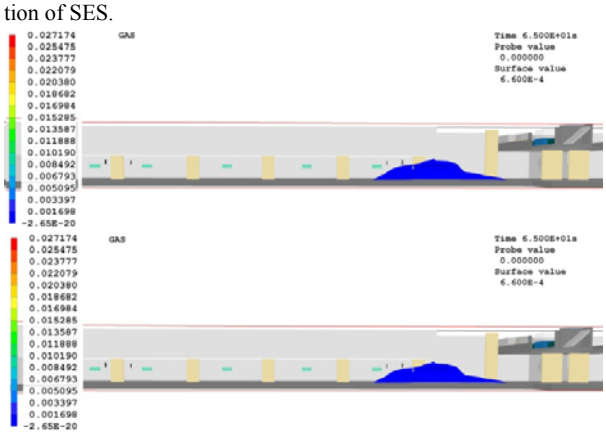

Figure 5: Iso-concentration surfaces of the contaminant at the time step corresponding to dispersion phenomena: (a) 7.5 s; (b) 65.0 s.

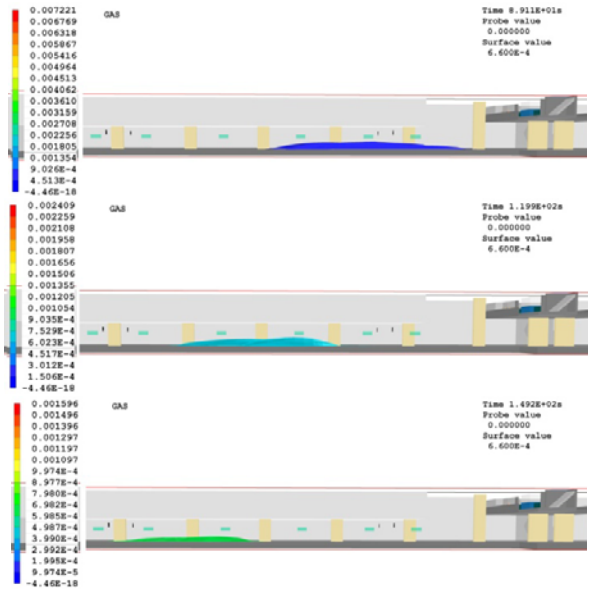

Figure 6: Iso-concentration surfaces of the contaminant at the time step corresponding to the first response: (a) 90.0 s; (b) 120.0 s; (c) 150.0 s.

In Fig. 5 and 6, the iso-concentration surfaces of the contaminant for several time steps are shown. These surfaces correspond to a mole fraction of 6.6 10^{-4}. It is easy to see that, before 65 s (Fig. 5 a, b), or when SES was not activated, the contaminant plume spread over the subway station freely, through diffusive and advective effects. Advective effects were due mostly to a nearby wall fan. After 65 s (Fig. 6), the simulation clearly illustrated the effectiveness of the SES for containing the contamination spread. The contaminant plume moved into the train tunnel on the left side, since the SES was activated with a negative x-direction velocity. It is noticeable that the scales in Fig. 6 are decreasing, suggesting that the SES action combines the displacement of the plume from the platform with the effect of diluting the plume with the passage of time. After 180 s, the iso-concentration surface was no longer present, which makes it obvious that the concentration of the contaminant over the platform was below the specified limit (a mole fraction of 6.6 10^{-4}). Since the contaminant agent is chlorine gas, it is possible to dispose of the agent onto the street. However, it is recommended to contain and decontaminate the gas plume (Fitch *et al*., 2003). In the present case, the train tunnel is long enough to be inserted into a gas treatment unit.

In case study 3, the contaminant was continuously released, beginning at 5 s and continuing until the end of simulation, which occurred at 240 s. The first-response time was assumed to be one minute, as in the previous cases. During this minute, the gas was dispersed by molecular diffusion and fan flow advection. Beginning after 65 s, the contaminant was extracted into the atmosphere through a set of corridor stairs. This condition is the boundary condition and was maintained until the end of the simulation.

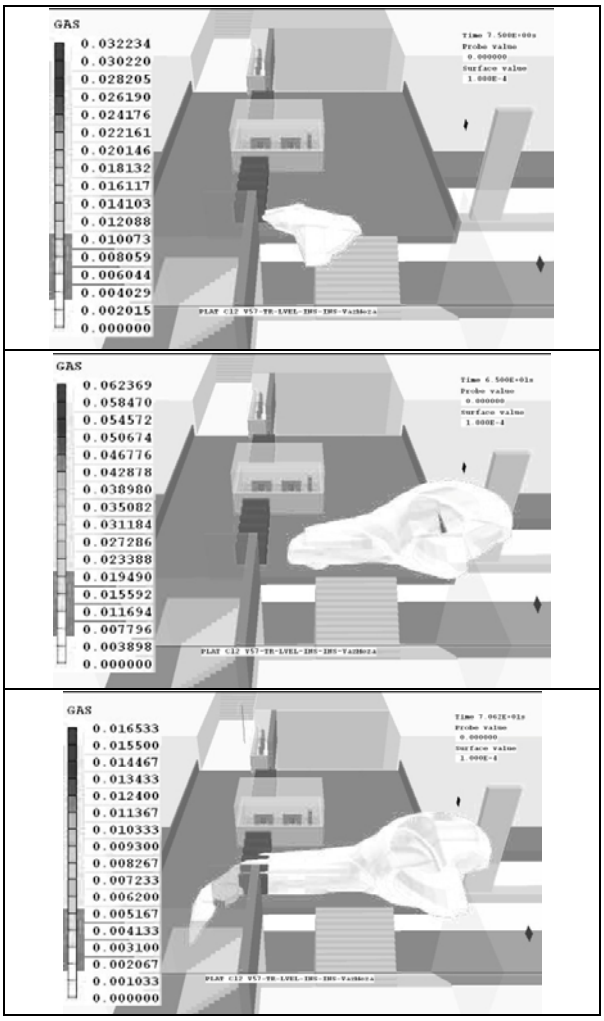

Figure 7: Iso-concentration surfaces of the contaminant at the time steps: (a) 7.5s; (b) 65.5 s; (c) 70.0s.

Figures 7 and 8 depict the iso-concentration surfaces of the contaminant during the simulation and indicate the lethal dose LD_{50}. It can be seen that until the time point of 65 s, the gas flowed slowly by molecular diffusion, as there was not significant advection from the small fans. After the SES was turned on, the gas was forced to the exit, and the steady state concentration increased after 180 s.

All of the present results are valid under the assumption that detection occurred one minute after contamination began. As discussed before, this may seem unrealistic, since there are no automatic detectors in the station. Under this assumption, the contaminant spread was contained by the SES activation, suggesting that the smoke extraction devices are efficient when activated very soon after the release. Therefore, an efficient sensor network is very important to control the dispersion of the contaminant.

The current recommendation to extract the agent into the street through the corridor stairs, according to our simulations, is not the best choice. Obviously, it would be a good idea if the agent is composed of smoke and fire, but the same is not true for a chemical contaminant. The simulation results point out that the flow has to be redirected to a gas treatment facility, which can be inserted in the train tunnel later.

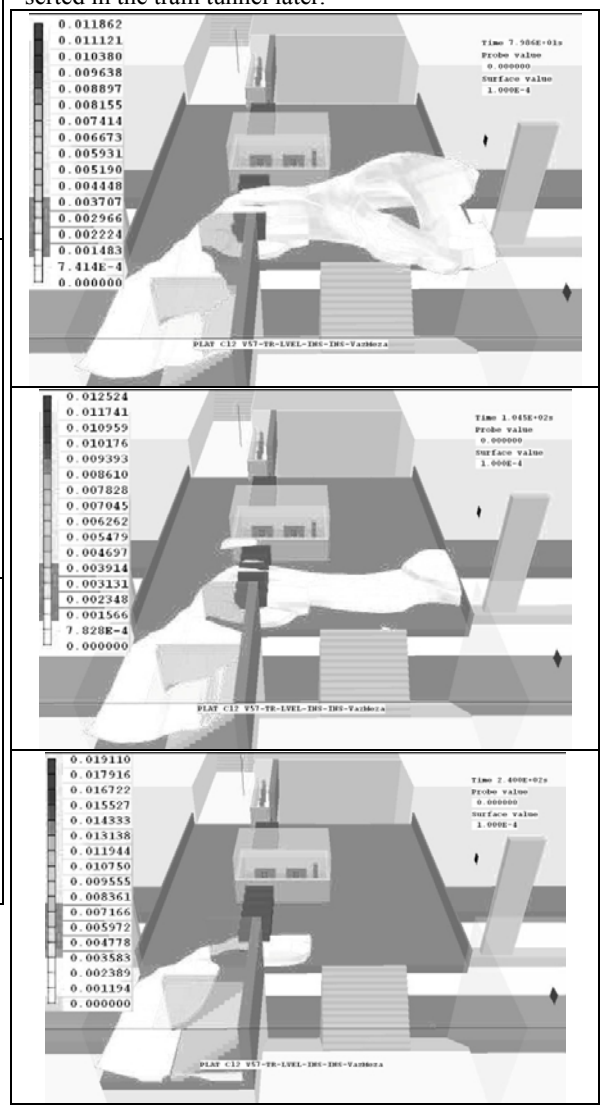

Figure 8: Iso-concentration surfaces of contaminant at the time steps corresponding to the first response: (a) 80.0s; (b) 105.0s; (c) 240.0s.

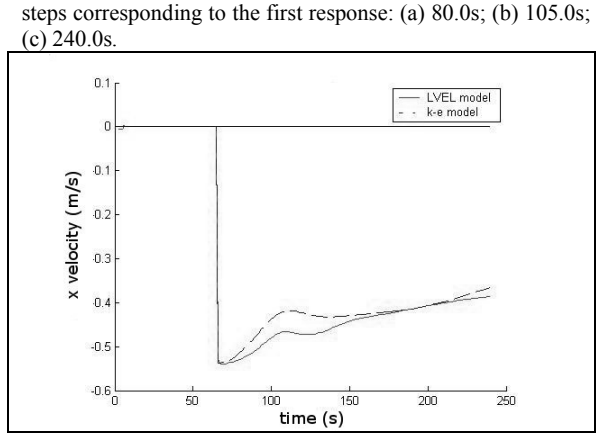

Figure 9: Velocity profile in the x-directions over time for one monitoring point.

In Fig. 9, a comparison between the x-direction velocities for the LVEL and κ-ε turbulence models is presented for one monitoring point. Similarly for the other fourteen monitoring points, there are no significant differences between the LVEL model results and the κ-ε model results.

If the LVEL turbulence model was used, the computing time was 80 hours. The κ-ε model was also applied since there are not experimental points, and a numerical validation was necessary. The computing time using this model was 120 hours. This time increment was higher than the others because there are other demands: 1- two additional equations were required to calculate the solution and 2- it is necessary to use an under-relaxation procedure.

IV. CONCLUSIONS

This paper addresses the simulation of a terrorist attack in a subway station. It uses PHOENICS commercial code to investigate the efficiency of subway smoke extraction equipment in containing the dispersion of a chemical contaminant.

In case study 2, the transient leakage of chlorine indicates that the subway's smoke extraction systems could control contaminant dispersion on the platforms, especially if the SESs are activated in the exhaust mode. The value corresponding to one tenth of the mole fraction of the LD_{50} of chlorine gas at atmospheric pressure and 298 K was set as the maximum allowable exposure for three minutes. Because a chemical contaminant may be extracted into the street, an undesirable consequence, we recommend that the flow could be redirected to a gas treatment facility, which can be inserted into the train tunnel.

In case study 3, the contaminant was continuously released on the mezzanine. If the agent was smoke, the current recommendation would be to extract the agent to the street through the stairs. The simulation results confirmed that another solution must be proposed for a chemical agent, since, with the current system, the chlorine gas plume goes through the stairway, a main evacuation route for people leaving the station. One solution would be to redirect the contaminant flow into a gas treatment facility existing deeper into the tunnel.

Finally, the present work has shown that CFD can be an excellent tool for mitigation and contingency planning of gas dispersion phenomena.

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