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Analysis of chlorine gas incident simulation and dispersion within a complex and populated urban area via computational fluid dynamics

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ABSTRACT

In some instances, it is inevitable that large amounts of potentially hazardous chemicals like chlorine gas are stored and used in facilities in densely populated areas. In such cases, all safety issues must be carefully considered. To reach this goal, it is important to have accurate information concerning chlorine gas behaviors and how it is dispersed in dense urban areas. Furthermore, maintaining adequate air movement and the ability to purge ambient from potential toxic and dangerous chemicals like chlorine gas could be helpful. These are among the most important actions to be taken toward the improvement of safety in a big metropolis like Tehran. This paper investigates and analyzes chlorine gas leakage scenarios, including its dispersion and natural air ventilation effects on how it might be geographically spread in a city, using computational fluid dynamic (CFD). Simulations of possible hazardous events and solutions for preventing or reducing their probability are presented to gain a better insight into the incidents. These investigations are done by considering hypothetical scenarios which consist of chlorine gas leakages from pipelines or storage tanks under different conditions. These CFD simulation results are used to investigate and analyze chlorine gas behaviors, dispersion, distribution, accumulation, and other possible hazards by means of a simplified CAD model of an urban area near a water-treatment facility. Possible hazards as well as some prevention and post incident solutions are also suggested.

Nomenclature

- ρ Density of the specific component
- μ Molecular dynamic viscosity.
- u Presents velocity component in corresponding direction.
- T Reynolds stress tensor
- Surain rate tensor
 Turbulent dissipation
- ${\mathcal E}_{
 m k}$ Turbulent kinetic energy
- P Pressure
- δ_{ii} Unit tensor (Kronecker delta)
- $C_{_{ai}}f_{_i}$ Adjustable constants which are obtained usually from data fitting

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1. Introduction

The importance of public health and safety has drawn more attention to environmental awareness concerning accidental or even intentional release of industrial toxic gases and wastes in crowded industrial sites or populated urban areas. Comprehensive studies of gas release and dispersion behavior of hazardous materials are the main characteristic of risk assessment. The release or the leakage of such hazardous materials may be a result of an accident in material storage, transportation, and application [1,2]. Chemical substances transported or used in urban areas are much more vulnerable to accidents than those in plants in remote locations. For instance, chlorine gas is transported in high pressure tanks (+2000 kPa) in liquid form. These chemical substances could be dispersed in densely populated areas such as metropolitan cities and cause horrific tragedies. Within the past few years, increasing concerns about a terrorist attack on strategic locations such as chemical plants have influenced public opinion about the issue. The strategic and sensitive location of Tehran, capital of Iran, adds to the importance of the issue.

Water-treatment facilities are one of the most strategic locations of every metropolitan because they provide

potable water. A recent terrorist attack by ISIS militants on the Fallujah water-treatment center in Iraq poisoned the city drinking water and a huge amount of chlorine gas was released into the air [1]. Thus, water-treatment facili ties could be potentially terrorist targets as they store and use huge amounts of chlorine. Furthermore, the Chlorine Institute estimates a chlorine tank terrorist attack could disperse a toxic cloud in an area as vast as 24 square kilo meters. The Naval Research Laboratory estimates this size of cloud could kill or injure up to 100,000 people in under a half hour. This might be the reason why chlorine gas has been used in many terrorist acts in Iraq [2]. Apart from these events, a very recent chlorine gas leak in the chlo rine injection pipeline in the fifth water purification station in the Fatemi Tehran Wastewater Treatment Plant injured some of the plant's workers [3].

Chlorine is a heavy gas, heavier than air, with a vapor density of 2.48 (air=1). It remains ground-level and is therefore more likely to be harmful to humans. The heavy gas cloud caused by the chlorine has the negative buoyancy which impacts and changes the behavior of the cloud when it is compared to a positively or neutrally buoyant cloud. Therefore, all these parameters must be considered when designing a model to predict any heavy gas behavior. Heavy gas dispersion modeling in a complex area is very sophisticated; it has been investigated in many researches around the globe from two points of view, safety and environmental issues. Some of the latest CFD works on gas dispersion modeling has focused on the effects of obstacles and barriers on gas concentration and transfer phenomena. When an urban area is being studied and a complex environment which has many buildings and structures surrounding the source of the chlorine gas are considered, the gas dispersion is greatly affected. Consequently, there might be stagnant areas and channels. To address such issues, this paper investigated the chlorine gas release or leakage from the Fatemi water-treatment facility in a 3D (three-dimensional) urban environment model with ANSYS CFX codes, which has been proven an accurate and reliable code in heavy gas dispersion scenarios [6-8].

This paper addresses the atmospheric elements and their impact on possible chlorine gas dispersion. These elements could be the buildings, physical barriers, wind, and air ventilation. In order to minimize the assumptions and reduce the computing cost, the environment of test subject is simulated under isothermal condition. A simplified CAD model of the area around the Fatemi water-treatment center was designed and meshed. After these steps, the model underwent several simulations using the computer fluid dynamic software (ANSYS CFX) in order to investigate the behaviors of chlorine gas in distinct scenarios. Afterward, the results obtained from the simulations were analyzed and discussed as risk assessment case studies. In order to reduce the probability of occurrence or at least reduce the impact of possible hazards, some suggestions are provided.

2. Background and history

odor, has been the source of many serious chemical accidents in the world. Many of these accidents caused a tremendous amount of damage to the environment and humans too. Chlorine gas incidents could be divided into the two main categories, indoor and outdoor. In recent years, the leading causes of these accidents have been chlorine leakage or spills from pressurized tanks, trains, and transportation trucks when human faults occur.

In December of 2011, an accident regarding a chlorine leakage in a public swimming pool poisoned at least 30 students in Ghasem Abaad, Mashhad [4]. A similar accident caused by a rusty pipe in the chlorine injector occurred at the Hootan swimming pool in Tehran. This incident caused human injuries, two of which were severe [5]. To date, one of the most horrendous accidents involving chlorine gas was the Graniteville train incident in United States. In this incident, a huge amount of chlorine gas was dispersed into the environment. This catastrophic event which happened on January 6, 2005, killed nine people and poisoned another 550. The economic aspect of this incident was also huge, as the Norfolk Southern Railway estimated the damage to be at least \$30 million [6].

These events and incidents highlight the importance of safety in areas in which chlorine gas is being used. Since it is impossible to prevent all of these types of accidents, it is important to understand the chlorine gas dispersion characteristics and its potential hazards.

There have been some field experiments covering this topic. The chlorine plume dispersion experiment done by Aurelia Dandrieux et al. was one such test. They used a chlorine release system and concentration sensors in their test sites to investigate an integral model and the Gaussian formulation. They found that the concentration predicted by a second approach is fairly close to their field tests. However, the integral model was not accurate enough and didn't match their experiments [7].

In another recent study done by Steven R. Hanna and his crew, the investigation of chlorine gas released from a train in an urban environment via Gexcon FLACS CFD solution was conducted [8].

In regard to enclosed areas, Paul Griffin et al. utilized CFD codes to simulate a gas release in the Sheffield city hall. A detailed design of the city hall was created with CAD and then CFD methods were used to calculate, estimate, and evaluate the ventilation rate [9].

3. Weather assessment, population and buildings density, area analysis, and geological data of the area

Tehran features a semi-arid, continental climate (Köppen climate classification: BSk). Its weather is mainly defined by its geographic location, with the Alborz Mountains to the north and the central desert to its south. Since Tehran covers a relatively vast area, the weather is often cooler in the hilly north than in the flat southern part of Tehran. The annual weather data for Tehran, which were recorded at the Mehrabad Airport weather station, can be observed in the following table:

Table 1. Annual climate data for Tehran- Mehrabad Airport [10].

	Record High °C	Avg. High °C	Avg. Low °C	Record Low °C	Precipitation mm	Avg. Rainy days	Avg. Snowy days	% Humidity	Mean monthly sunshine hours
_	44	22.68	11.75	-15.1	232.8	76.4	12.3	41.1	3030.2

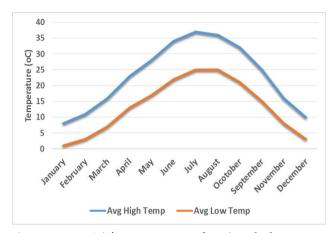


Fig. 1. Average High/Low Temperature for Tehran [11].

Tehran has a total area of 750 km², an average elevation of 1200 m, a population of 11 Million in 2006 (as noted by www.Tehran.ir), and a population density of 10,327.6/km² [12].

The water-treatment facility analyzed and investigated in this study is one of the very first water-treatment facilities in Iran and was built in 1955. Water for this facility is provided by the Karaj River. This facility provides potable water for the western side of Tehran. This facility is located in a very crowded and dense area of Tehran in terms of both buildings and population. It is also located to the NE of Laleh Park. The dominant wind direction in Tehran is from the west, and the mean average wind flow speed is 5.5 meter per second [13]. Other sources note that the mean average wind flow speed of 3.1 meter per second was observed for the last 10 years in Tehran and the highest recorded wind speed was 24 m s⁻¹ in 2011. Furthermore, the mean average humidity in this 10 year period was 35% and the air pressure was 1 atm or 101 kPa [14].

4. Validation and basic theory of CFD

As of today, many approaches were developed for the investigation of gas behaviors. One of these approaches is "Computational Fluid Dynamics" (CFD). This method can be used in achieving numerical solutions and algorithm for ventilation and gas dispersion modeling for both offshore and onshore plants [15]. CFD solutions are becoming more and more common. The NORSOK (Norsk Sokkels Konkuranseposisjon) standard number Z-013 defines the possible usages of CFD in its realistic approach to risk assessment and preparedness [16]. Gas leakages, ventilation assessments, and gas dispersion as well as gas explosions are investigated through suitable and real scenarios via this method.

Computational fluid dynamics assess the simulation of sophisticated physical processes and cases, describing heat and mass transport phenomena (conservation equations for mass, momentum and enthalpy) with fully developed mathematical models. As for turbulent conditions, the CFD solution such as ANSYS CFX also uses the K-epsilon model. This model is a two equation model which provides a comprehensive description of turbulence fluid behavior by the means of two transport equations (PDEs).

The two-equation model of the K-epsilon is written as following [17]:

$$\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_j k)}{\partial x_j} = P - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_i}{\sigma_k} \right) \frac{\partial (k)}{\partial x_j} \right] + \rho L_k$$
 (1)

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho u_{j}\varepsilon)}{\partial x_{j}} = C_{\varepsilon} f_{1} \frac{\varepsilon}{k} P - C_{\varepsilon} f_{2} \frac{\rho\varepsilon^{2}}{k} P + \frac{\partial}{\partial x_{j}} \left[\left(\mu + \frac{\mu_{i}}{\sigma_{\varepsilon}} \right) \frac{\partial(\varepsilon)}{\partial x_{j}} \right]$$
 (2)

Where:

$$P = \tau_{ij} \frac{\partial u_i}{\partial x_j} \tag{3}$$

$$\tau_{ij} = \mu_t \left(2S_{ij} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \, \delta_{ij} \tag{4}$$

$$S_{ij} = 0.5(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})$$
 (5)

And the turbulent eddy viscosity can be computed via:

$$\mu_{t} = C_{\mu} f_{\mu} \frac{\rho k^{2}}{\varepsilon} \tag{6}$$

Where ρ is the density of the specific component and μ is its molecular dynamic viscosity.

ANSYS CFX allows for computational simulations of atmospheric dispersion of gases around both an isolated cubical obstacle and an array of obstacles; as a supporting case, it also matches the Thorney Island and Kit-Fox experiments.

The turbulence model used in those papers was k-epsilon, which has been tested, evaluated, and validated by many researchers and scientist [6,8,22]. The interpretation and scale-up from the CFD experiment and Kit-fox observation is possible considering the cubical obstacles as buildings and other barriers as the arrays of obstacles in a city [18]. According to many research papers and experiments, gas dispersion simulations in complex and crowded environment are feasible and very effective via ANSYS CFX codes. Moreover, defining the problem correctly and precisely in the early stage of the simulation in the software parameters is considered crucial in order to achieve an acceptable result [8,22,23].

5. Area Model Detail

For this article, an area of almost 1 Km radius around the mentioned water treatment facility was traced and modeled using Microsoft Virtual Earth (Bing Maps Satellite images) satellite images in order to have a simplified 3D model of the area. Initially, the area satellite image was extracted from Bing Maps by using SAS Planet in order to have a high-quality 70 Mpx satellite image of the area in one image. The 2D line tracing was done in Rhinoceros 5.0 software using Rhino Script in order to do the image processing, buildings, and other obstacles tracing. The model accuracy, precisions of image tracing, and modeling gradually decreased the further the distance from the water-treatment facility. The more distance from the chlorine gas leakage source, the geometrical detail becomes less important in the matter of gas dispersion incidents. Moreover, the 3D model of this area is being simplified, made less complex and lighter for the meshing stage and more importantly in the CFD solving and simulation stage. In order to speed-up the area 3D modeling process, an average building height of between 20-40 meters is utilized randomly using the Rhinoceros script for each building and obstacle. Several random heights in the 3D models of the area were tested in chlorine gas dispersion scenarios, and no significant difference and changes in the CFD results were observed. This proves that the exact height of the buildings and obstacles are not important. In addition, nearby buildings are treated as one unified obstacle in order to simplify the whole process. Furthermore, to obtain a more precise model and better calculation results, the exact height of important and tall buildings were entered manually in the process of the 3D modeling of the area. Also, DEM (Digital Elevation Model) was used in order to add precision to the calculation and modeling. Another important factor of the 3D model is that the east side of the water-treatment facility is more detailed than the west side. This is because the dominant wind flow direction is from the west in this area, and the west side of the facility geometry became less important. All of these assumptions were made to minimize the computing costs and to make the CFD calculation on this scale possible. In order to simplify the problem, the trees and other vegetation have not been considered in the modeling as the obstacles because most of the trees in this area and in this case are located on the west side of the facility. However, in order to consider their effects, the turbulence level is defined as medium. Thus they can be neglected in order to simplify the problem. The entire area covered has a dimension of 2353.75 x 1725.6 meters (4061631 square meter), and it has (bounding box of the area) an approximate volume of 513376794 m³. The entire area is covered with 423 individual obstacles. In order to consider the effect of the buildings in that specific area, spacing's were adopted around the model.

Preparation of the city model for simulations was done in two stages:

- 1- Tracing and designing of the city model in CAD software using geographical (DEM) and satellite images
- 2- Sufficient and optimized meshing of the model for the simulations

In Fig. 2, an overall view of the water-treatment facility and its surrounding area model is presented. It contains a sufficient amount of details which is adequate for these types of simulations on this scale.

In order to determine the behaviors and characterizations of the air ventilation in the area, a CAD model was designed in Rhinoceros software. It was meshed in tetrahedral mesh format in an ANSYS Workbench, which consists of 44060 nodes and more than 214540 elements, used in ANSYS CFX. This amount of detail in a CAD model not only conserves a sufficient and acceptable amount of accuracy, it also reduces the processing time and lowers the computer resource usage. Higher amounts of elements and mesh where considered, but there were no significant changes in the results.

Computational resource specifications were, Core i7-3612QM (Quad-Core processor each core at 3.1 GHz) as the main processor. The amount of physical rams which was used by the main scenarios was around 5.2 GB.

6. Analysis of gas dispersion in different scenarios and circumstances in the area

In order to minimize the assumptions and hypothetical specifications, and further ensure relatively accurate simulation, meteorological data are used including wind flow speed and direction profile in boundary layers. As previously mentioned, the dominant wind profile in this area flows from the west with the average speed of 5.5 m s⁻¹.

In order to investigate the safety of the area in various circumstances in which chlorine gas had been leaked and dispersed from a storage tank or a pipeline, different hazardous situations were carefully chosen and defined in the ANSYS CFX. First of all, steady-state CFD results are acquired by simulating a typical day without any occurrence of leakage under weather conditions with an average temperature of 25 °C and wind flows at 5 m s⁻¹.

In Fig. 3, simulated wind-flow is illustrated in our urban area from a perspective angle in order to give an idea regarding the flow behavior. Later, the results from the steady state condition shown in Fig. 3 are used as initial conditions in other scenarios.

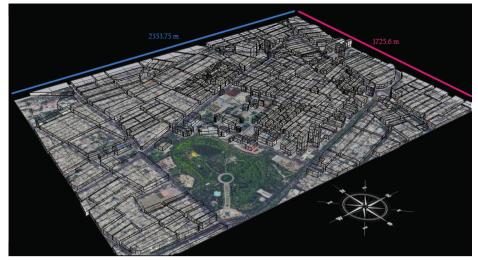


Fig. 2. Area overall view.

In order to decrease the calculation time, these steadystate simulations and its acquired results are used as initial condition in transient and unsteady state conditions Two scenarios were properly investigated: One in which a huge leak occurs and the wind flow is from the west; The other is a relatively smaller leak but the wind flow is not only from the west but a little from the south.

6.1. Scenario 1- Massive chlorine gas leakage and dispersion in the facility

A hypothetical scenario is considered. Following an explosion in a chlorine storage area, a huge amount of chlorine gas is leaked and dispersion has occurred. The chlorine is being released into the open-air with a mass flow rate of 6 kg s⁻¹. This leakage continued for 15 minutes at the same rate until engineers were able to stop it. Wind and natural air ventilations are rapidly scattering, expanding, dispersing, and leading the leaked chlorine gas cloud to the east side of the facility because the wind flows from the west.

The specifications and details for Scenario 1 are:

- -Wind flow velocity in the area is 5 m s⁻¹ from the west (constant profile)
- -The other side of the bounding box of the area is considered as open (as its boundary type condition)
 - -Weather temperature is 25 °C (a normal day condition)
 - -Air pressure is considered 1 atm (101.325 kPa)
 - -Unsteady-state conditions are considered
- -Chlorine gas is released to the open-air at 6 kg s⁻¹ for 15 minutes from the liquid chlorine gas storage
- -The simulation area has the dimension of 2353 x 1725 m^2 with almost 510 million cubic meters of air

One virtual sensor is placed 690 m away from the east side of the facility (Fig. 4) at an elevation of 1.50 m in the Vali-Asr Street in order to record chlorine gas concentration after the chlorine gas incident has occurred.

The results are as follows:

As it is known, the IDLH concentration of the chlorine gas

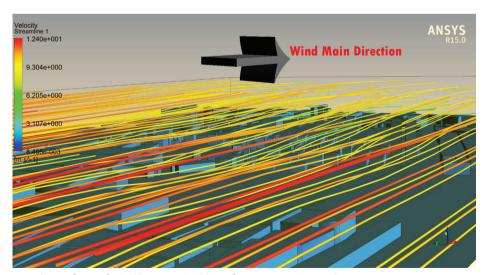


Fig. 3. Air flow stream lines of 5 m $\rm s^{-1}$ wind between buildings from perspective angles.



Fig. 4. (Point A): Virtual sensor position 690 m away from the facility.

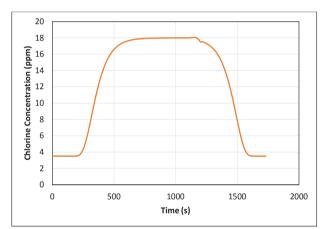


Fig. 5. Chlorine gas concentration in point A of Fig. 4 vs. time.

is 10 mg L⁻¹. After almost 5 minutes, the chlorine gas concentration will reach-up to the IDLH level in point A away from the facility. The chlorine gas concentration level keeps growing until it nearly reaches 18 mg L⁻¹ at point A. Such a high concentration of chlorine gas in the air in this densely populated area could endanger hundreds to thousands of individuals in the east side of the facility. Moreover, because chlorine gas is heavier than air, some of it will remain in the leakage area in the facility for a relatively extended period of time; it will not be scattered and dispersed by the wind. So even after a long period of time, the engineers and attending rescue teams at the site will need to use suitable gas masks.

Fig. 6 presents the IDLH concentration of the chlorine gas cloud (10 mg L⁻¹) in the form of an Iso-surface geometry 60 seconds after the incident.

Furthermore, Fig. 7 shows the same concentration gas cloud (IDLH concentration) after 800 second following the incident. As it is observed, the chlorine gas is dispersed in an almost straight line in this situation.

As this case is more concerned with the possible human

casualties, all people living on the east side of the water-treatment facility should be immediately evacuated to higher grounds. The north or the south could be considered as safe zones for the evacuation. Since most of the chlorine travels to the east with the wind, it is a wise choice. As previously mentioned, chlorine is heavier than air so it remains in the lower grounds. Therefore, it will possibly be more dangerous for the people in the streets. Therefore, moving to higher grounds is highly recommended for the people in the area.

6.2. Scenario 2- Light unsteady chlorine release

In the following scenario, another chlorine gas leakage is investigated. The leakage rate is as high as 1 kg s⁻¹ for about 15 minutes. The chlorine storage tank contains pure chlorine gas (Cl_2). The wind in this scenario is mainly from west, and it has a logarithmic profile. Wind condition should be considered by the reduction of wind speed at the surface level because of the surface roughness. The wind speeds are mainly provided at a known height (Reference height is mostly 10 m above the surface), then the wind velocity profile could be written as a logarithmic correlation as follows [19]:

$$u_{2} = u_{1}\left(\frac{\ln\left(\frac{h_{2}}{z_{0}}\right)}{\ln\left(\frac{h_{1}}{z_{0}}\right)}\right)$$
 (7)

Where u_2 is the wind velocity at the desired height (h_2) and u_1 is the reference wind speed at a specific height (h_1) . As z_0 presents the roughness length and simulation takes place in an urban area with tall buildings and skyscrapers, the value for roughness length or z_0 can be considered 1.6 as it is recommended by the roughness length table [19].

The height vs. wind velocity by this formula is illustrated in Fig. 8:

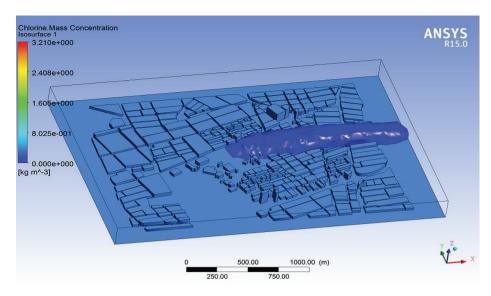


Fig. 6. Chlorine gas cloud with the IDLH concentration after 60 s following the incident in the area.

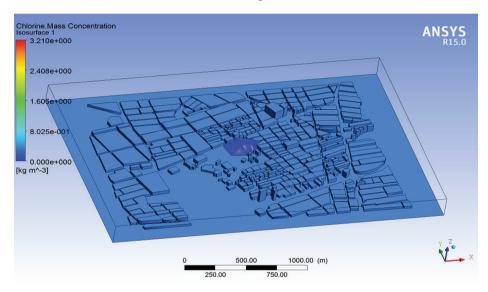


Fig. 7. Chlorine gas cloud with the IDLH concentration after 800 s after the incident in the area.

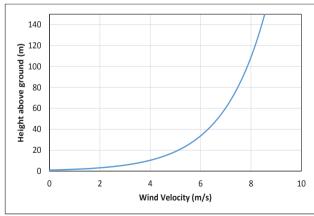


Fig. 8. Wind profile.

Furthermore, the wind streamlines can be seen in Fig. 9.

In Scenario 2, the parameters are specified as follows:

- -Wind from the west by a logarithmic profile with the mean average of 5 m $\ensuremath{\text{s}}^{\text{-1}}$
- -Weather temperature is 25 $^{\circ}\text{C}$ and the air pressure is 1 atmosphere
 - -Transient conditions are considered for about 1 hour
- -Continuous gas leakage consists of 100% volume fraction of chlorine with overall mass flow rate of 1 kg s $^{\text{-}1}$ for about 15 minutes

As mentioned before, the IDLH value for chlorine gas is 10 mg $L^{\text{-}1}$. As in the previous scenario, a chlorine gas cloud with a concentration of more than 10 mg $L^{\text{-}1}$ must be considered. In the following figure, a chlorine gas cloud for 10 mg $L^{\text{-}1}$ is shown after 12 minutes:

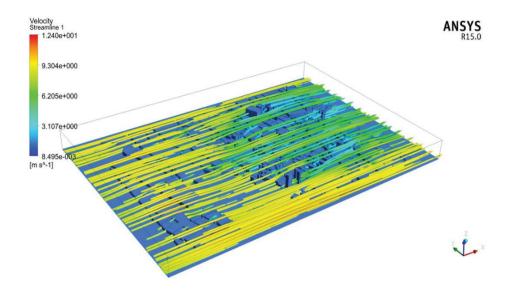


Fig. 9. Wind flow lines around the facility.

There is absolutely no trace of chlorine in the city environment with a concentration of 10 mg L^{-1} within one hour of simulation. Even lower concentrations of chlorine, like 5 mg L^{-1} , are diluted very quickly. The following chart shows the chlorine gas concentration in Vali-Asr (Point A) which is located within the wind flow direction:

As seen in the chart, the chlorine gas concentration in this area, which is fairly close to the incident site, would never exceed more than 5 mg L⁻¹; and after almost 20 minutes, it reaches zero.

As observed in the simulation results of this scenario, there should be no serious hazardous event in the city at this leakage rate. However, the facility's environment remains toxic and must be considered as a red-zone because

of the presence of significantly contaminated air. All individuals must evacuate the facility until further notice. The main concern in this case is the inside of the facility and its workers. Therefore, precautionary procedures must be executed in order to reach safe levels of chlorine gas concentration in the facilities.

7. Results and discussion

As illustrated in the simulated chlorine incident, the most vulnerable targets are the people living in the eastern part of Tehran as the gas cloud moves in this direction. In the case of a terrorist attack or an accident at the Fatemi water-treatment facility or other facilities which store high



Fig. 10. Chlorine gas cloud of 10 mg L⁻¹ after 1000 seconds (dark blue polygon in the middle).

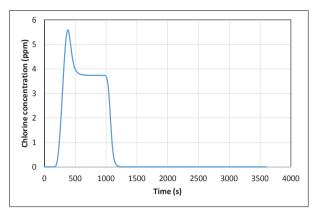


Fig. 11. Chlorine gas concentration in Vali-Asr (Point A).

amounts of chlorine gas, horrific scenarios might happen because these areas are densely populated. The areas of Pasdaran and Motahari would be affected and the gas clouds might reach Tehran-Pars or the Narmak region. Thus, safety precautions should be put in place to prevent serious consequences. Furthermore, increased security and safety measures in sensitive locations, like chlorine storage sites, could be a wise approach in order to prevent accidents or terrorist attacks.

More to the point, chlorine has been used by many terrorist organizations [20]. Therefore, government agencies should practice caution in regard to urban areas in Tehran in which chlorine is used as these locations could be potential terrorist targets and attacks on them could be catastrophic.

8. Conclusion

It was observed that utilizing ANSYS CFX code and CFD simulations in hazard simulation on a large scale can be considered as a very helpful and cost efficient approach not only in health and safety case studies but also in pre and post urban planning. Once again, CFX in this case shows significant precision even on these massive scales. These types of simulations could be considered as a beneficial, affordable, and accurate solution compared to experimental and laboratory methods such as analyzing expensive city models in a wind tunnel. This available know how is advantageous in order to suggest any necessary changes in the initial urban planning designs so as to promote a city with better and more effective natural air ventilation. This could also lead to less air pollution in the future. Furthermore, CFX could compute and predict not only chlorine gas, but also other potentially hazardous gas concentrations and dispersion after a gas leak incident. These simulations could also be used to investigate the gas cloud dispersion in distinct scenarios and various weather conditions in different seasons in either steady or unsteady conditions. Simulation results could be used by rescue teams like the fire department, environment agency, civil engineers, and many other departments and organization within the city. Additionally, a gas dispersion model can be animated and viewed in order to gain better insight of how the gas is scattered in a hazardous situation thus helping to educate and prepare the rescue teams before facing real dangers. Future work and improvements may include: adding constrains of heat transfer equations and investigation of how their presence impacts on the results; analysis of humidity effects; doing the simulations for specific season; and comparing the results for various models with various levels of details.

References

- [1] Lisi, R., Maschio, G., & Milazzo, M. F. (2007). Terrorist actions in the transport of dangerous goods in urban areas. In *IChemE symposium series* (No. 153).
- [2] Maschio, G., & Milazzo, M. F. (2008). Risk evaluation of terrorist attacks against chemical facilities and transport systems in urban areas. In *Resilience of Cities to Terrorist and other Threats* (pp. 37-53). Springer Netherlands.
- [3] Alalam News Network. (2014, June 13). News. Retrieved from Alalam News Network: http://fa.alalam.ir/news/1602445
- [4] The New York Times. (2007, February 22). World News. Retrieved from The New York Times: http://www.nytimes.com/2007/02/22/world/middleeast/22iraq.html
- [5] Tehran Province Water and Wastewater. (2014). *News and event*. Retrieved from Tehran Province Water and Wastewater: *http://tpww.co.ir*
- [6] Gavelli, F., Bullister, E., & Kytomaa, H. (2008). Application of CFD (Fluent) to LNG spills into geometrically complex environments. *Journal of hazardous materials*, 159(1), 158-168.
- [7] Freeman, M., Spencer, R., & Huber, A. (2013). Scientific Visualization for Micro-Scale Modeling of Airborne Pollution in Urban Areas. EPA.
- [8] Kashi, E., Shahraki, F., Rashtchian, D., & Behzadmehr, A. (2009). Effects of vertical temperature gradient on heavy gas dispersion in build up area. *Iranian journal of chemical engineering*, 6(3), 26-45.
- [9] Jam e Jam. (2012 Dec 16). Poisioned students with Chlorine in the swimming pool (in persian). Retrieved from http://www1.jamejamonline.ir/papertext.aspx?news-num=100830536776.
- [10] FardaNews. (2012, Jan 25). 11 Injured in Chlrone gas incident in Hootan Swimming pool in Tehran. Retrieved from http://www.fardanews.com/fa/print/184580
- [11] Dunning, A., & Oswalt, J. (2015). Train wreck and chlorine spill in Graniteville, South Carolina: Transportation effects and lessons in small-town capacity for no-notice evacuation. *Transportation Research Record: Journal of the transportation research board*, 130-135.
- [12] Dandrieux, A., Dimbour, J. P., & Dusserre, G. (2006). Are dispersion models suitable for simulating small gaseous chlorine releases?. *Journal of loss prevention in the process industries*, 19(6), 683-689.
- [13] Hanna, S. R., Hansen, O. R., Ichard, M., & Strimaitis, D. (2009). CFD model simulation of dispersion from chlorine railcar releases in industrial and urban areas. *Atmospheric environment*, *43*(2), 262-270.
- [14] Gilfrin, P., & Hatfield, E. (2005). Visualizing Sheffield

- City Hall Airflow. AEC Magazine, 23, 25-26.
- [15] Qiao, A., & Zhang, S. (2010). Advanced CFD modeling on vapor dispersion and vapor cloud explosion. *Journal of loss prevention in the process industries*, 23(6), 843-848.
- [16] World Weather. (2014). Tehran Monthly Climate Average. Retrieved from http://www.worldweatheronline.com/Tehran-weather-averages/Tehran/IR.aspx
- [17] Info. (2010). Tehran City Information. Retrieved from. Retrieved from http://www.city-infos.com/.
- [18] Municipality. (2012). Retrieved from http://www.teh-ran.ir/Default.aspx?tabid=117.
- [19] Wolfram. (2014). average wind speed in Tehran. Retrieved from http://www.wolframalpha.com/in-put/?i=average+wind+speed+in+Tehran
- [20] International Association of Oil and Gas Producers. (March 2010). *Risk Assessment Data Directory; Consequence modelling*. OGP.

- [21] NORSOK Standard. (2001). Risk and emergency preparedness analysis. *Norwegian Technology Standards Institution, Oslo, Norway*.
- [22] Chien, K. Y. (1982). Predictions of channel and boundary-layer flows with a low-Reynolds-number turbulence model. *AIAA journal*, *20*(1), 33-38.
- [23] Hoi, Y., Woodward, S. H., Kim, M., Taulbee, D. B., & Meng, H. (2006). Validation of CFD simulations of cerebral aneurysms with implication of geometric variations. *Journal of biomechanical engineering*, 128(6), 844-851.
- [24] Mirzaei, P. A., & Haghighat, F. (2012). A procedure to quantify the impact of mitigation techniques on the urban ventilation. *Building and environment*, 47, 410-420.
- [25] Carruthers, D. (2003). Handbook of Atmospheric Science: Principles and Applications. Blackwell.
- [26] PBS. (2012). *Inside Al Qaeda*. PBS. Retrieved from http://www.pbs.org/wgbh/pages/frontline/shows/network/algaeda/manual.html