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CFD Analysis of Indoor Chlorine Gas Dispersion Storage: Temperatures, Wind Velocities and Ventilation Effects Studies

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The Chemical products factories encounter inherent environmental risks in the process. The indoor release of hazardous chemical gases that are heavier than the air is nowadays a special subject for scrutiny because the dense clouds of the gas have a tendency to insist on the ground level or near the human breath level, causing fatal injuries or other potential health threats to human beings. In this study, a computational fluid dynamics (CFD) code FLUENT was employed in order to model the accidental indoor dispersion of a dense gas (chlorine) from a small undetected leak in an indoor industrial environment. Furthermore, the effects of different temperatures, wind velocities and ventilation on diffusion of chlorine are investigated in this paper. Results of the simulations represented that the chlorine gas dispersion would behave like the liquid and currents on the floor. It was also found that the chlorine concentration above the ground level increased slowly. Showing the effects of various temperatures and wind on spreading the dense gas will help to better identify the potential risks. In this research, the effects of the environmental situations with the release and spread of chlorine in the indoor space were meticulously investigated.

Keywords: CFD, Indoor Environment, Dense gas Dispersion, Various Temperatures and Wind Velocities, ventilation

INTRODUCTION

There are some challenges in the workplaces that one of the most important of them is to protect the workers in factories or people who are living near the industrial cities against toxic, flammable, and hazardous substances such as chlorine, asbestos, and so forth that are produced or used in various industries. Risk assistant of the hazardous gas dispersion is a significant task in the safety process since this scenario can lead to great results: the cloud of the toxic and hazardous heavy gas can be moved by wind to remote places and keep concentrated high enough to illustrate a hazard for human health and environment (Potinggia *et al*, 2009).

Chlorine is a great antiseptic bleaching agent and it is solvent as well. Having two forms normally the liquid and gas, chlorine is a toxic material which brings about numerous hazards. In details, it can cause death or serious injuries if suitable safety measures are not taken, among which an appropriate room with ventilations, alarms, gas detectors, and other necessary equipment for keeping cylinders or tanks (Anonymous, 2006). In order to protect the people who have a direct contact with the chlorine equipment or live next to it, governments should be required to expand and perform safety, health, and environment instructions (OHSAS18001) in the industrial places. Chlorine is used in various industries for manufacturing such as the chemistry and plastics productions, pharmaceuticals, paper bleaching, water purification, and so on (Winder, 2001).

Chlorine gas is 2.5 times heavier than the air at a normal atmospheric temperature and pressure while it has a propensity to downhill. Wind and climate will cause chlorine to diffuse in all directions (Anonymous, 2006). The exposure to chlorine happens in different situations. The cl_2 exposure standard is between 0.5 to 1 ppm (Winder, 2001). According to the NIOSH (National Institute for Occupational Safety and Health in the United States) standards, any exposure further than 10 ppm is capable of making serious hazards for the life and health of the humans and the environment.

These gases are typically stored in the liquefied state at the ambient temperature in exceedingly pressurized vessels. In case an accident occurs while the stored gas is abruptly depressurized the consequential jet will entail a gaseous vapor phase as well as a liquid phase encompassing the particle droplets melded with air. Numerous models could be employed to envisage the released gas’s concentrations while the acquired values can be employed for the hazard and risk assessment surveys or being used by the authorities (e.g. fire department), especially when an accident occurs (Kiša and Jelemenský, 2009).

Modeling the dispersion of gases is a critical step in the risk assessment. The base of most of famous modeling for traditional gas spreading models is the Gaussian distribution that has been improved for puff or plume diffusion of hazardous gases into the air (Siddiqui, et al 2012). In the recent years, the computer software has made a great evolution in the gas diffusion simulations: for instance, one of the methods for modeling the gas dispersion is the computational fluid dynamic (CFD) technique. Recently, to examine a quantity of accident scenarios, some robust simulation tools like the ones revolving around the computational fluid dynamics (CFD) have been given attention. The advancement in the scenarios in the outside environment has progressed so that it would be possible to make rather precise prophecies on the release patterns and their results. This is indeed possible even in complex scenarios (Potiggia *et al.*, 2011).

The basic equations which explain the mass conservation, momentum and energy balance in the CFD can be numerically solved for a certain flow domain, as well as initial and boundary conditions. It is possible to find the temporal and spatial evolution of the concentration field for various species through solving a species transport equation on a computational grid. It could be later utilized for more precisely specifying the three-dimensional turbulent dispersion effects in an indoor environment on the spreading pattern of a dense toxic gas and the concomitant risks. In the present study, this computational analysis is applied to the spreading of chlorine in an indoor environment and the benefits of this approach are emphasized (Siddiqui *et al.*, 2012).

In this study, we focused on release of dense gases such as chlorine to the atmosphere and exhibited the effects of various temperatures and wind velocities on the diffusion of heavy gas in small indoor environments. Recently, attempts to model such scenarios using CFD and related techniques (Siddiqui *et al.*, 2012). The significant objective of this study is to develop a CFD base model for forecasting the results of the accidents of the chlorine release in a small storehouse in various situations and investigated the effects of ventilation on Cl_2 diffusion in the air.

The remainder of the current paper is organized as follows. The validation of the model is described in section 2. The physical problems, chlorine room dimensions and details of the Computational fluid dynamic (CFD) simulation are represented in section 3; also, the results and discussions of the effects of various temperatures, wind velocities, and ventilation are described in the next section.

VALIDATION OF THE MODEL

It was possible to perform the validation of the computational model through establishing a comparison between the simulation results for both spreading and dispersion of Freon 22 accomplished in a 3D test room and the results of the experimental surveys by Gilham *et al.*, (1997). The results indicated that a liquid-like stratification effect existed in the spreading while the results proved to be in good qualitative agreement with the experimental data (Gilham *et al.*, 2000).

According to the experimental graph that it is shown in figure 1, after 300 seconds the concentration of CO_2 was about 20 % while the CFD simulation showed it to be near 18%. Also, both graphs indicate a gradual increasing trend.

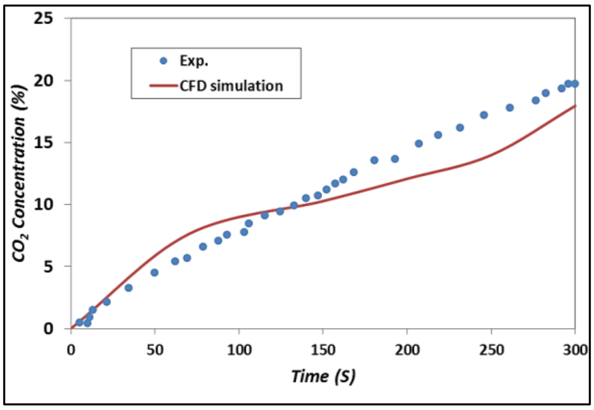


Fig. 1: The comparison between the experimental and cfd simulations

As a consequence, the computational model for the dense gas dispersion encompasses the subsequent elements:

- RANS-based governing equations with the k–ε turbulence model.
- Assessment of the local, sudden concentration of the dense gas species of interest by solving the scalar transport equation for the species.
- Making use of a favorable gas law-based equation of state to appraise the pertinent thermophysical characteristics of the gaseous mixture (Siddiqui *et al.*, 2012)

The details of the chlorine diffusion scenario is discussed in the following sections.

COMPUTATIONAL FLUID DYNAMICS (CFD)

In this paper three scenarios are introduced: the first scenario surveys the effects of different temperatures on the diffusion of chlorine in the indoor environment. The second scenario describes the effects of various wind velocity and temperatures on the gas dispersion, and the last scenario shows the Cl_2 spread in the indoor environment when the ventilation is working.

The Physical Problem

It needs to be asserted that the commercially available computational fluid dynamics (CFD) code FLUENT has been employed so far in several accident scenarios (Gilham *et al.*, 1997, Gilham *et al.*, 2000, Garcia *et al.*, 2008, Cheng *et al.*, 2009), . The simulation results in this research show the effects of the temperature, wind velocity, and ventilation on the dispersion of chlorine gas in the indoor environments that include a chlorine tank in the storage. The storeroom dimensions were 5m×4m×3m and it had two windows (W1 & W2) and a big door (D1) in the current research. The geometries of an intermediate storage tank (T) included the Length 118 Inches, the tank diameter 48 Inches, and the pipe diagonal 2 Inches. Also, the distance of pipe to the center of the circle is 20.5 Inches as shown in Figure 2.

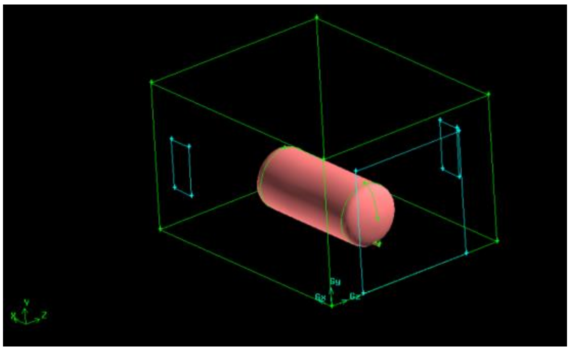


Fig. 2: The environment indoor

Two intermediate chlorine cylinders (C1 & C2) and intermittent storage room for chlorine in order to keep the compress cylinders (B1) and two ventilations on the wall that ingress vent (V1) were installed on the left wall and the exhaust vent (V2) set up on the side of the opposite wall with the diameter of 20 cm was installed on the walls (left and right) to remove the vapors released accidentally during the normal operation and all were designed in the ventilation simulation scenario as shown in Figure 3.

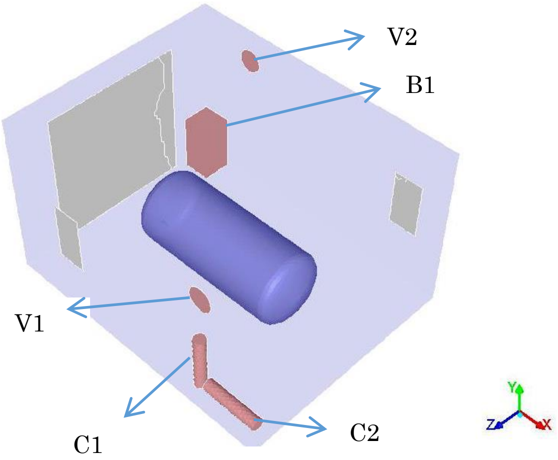


Fig. 3: The ventilation system

Details of The Simulations

Chlorine is an extremely toxic heavy gas. The critical concentration of chlorine for exposure limits begins from 10 ppm (Schmittinger, 2000) and a small release from the source is enough to exceed this level; According to this fact, the scenarios presumed in the present paper dealt with an incident of small leakage of chlorine from the pipe attached to the tank, by a joint failure. Also, it is supposed that the leakage is little enough that it has not been detected by the violation of mass balance. The mass flow rate of chlorine of the order of 0.01 kg/min was taken into account as the source release rate while hypothesizing a crack length of 10% of the pipe diameter and a crack width of 0.01 mm. It is presumed that a cloud of chlorine vapor will be formulated at the leakage site due to depressurization once the fluid exiting the crack. The computational model introduced previously was employed to make predictions on the spatio-temporal variation in the concentration of dense chlorine gas after the accidental release. The commercially available CFD code FLUENT, being employed in some accident scenarios surveyed through studies such as by Gilham *et al.* (1997), was employed in the current research.

In the first simulation all the doors and windows were closed and the temperatures were changed in 270 K, 297 K and 315 K while during the second scenario the windows were left opened: thus, there were wind velocities assumed at $1\,ms^{-1}$, $3\,ms^{-1}$ and $5\,ms^{-1}$ while the temperatures of the room fluctuated between 270K, 297K and 315K in all the velocities, respectively. In the third scenario all the doors and windows are closed and the fresh air goes in at identical flow rates via the ingress vent (V1) and at the determined rate of 3 m/s while it exists from the exhaust vent (V2), which is determined as the pressure outlet limits. It is assumed that the flow is turbulent and the *k*–*ε* turbulence model was accordingly employed. Taking into account the domain size, the wall functions were utilized at all the walls to maintain the grid size at controllable levels. Because the velocities in the current research are rather slight and no heat transfer was regarded, it was anticipated that no particular wall-induced impacts (like relaminarization under intensely accelerating circumstances) will be experienced. Consequently, a standard wall function

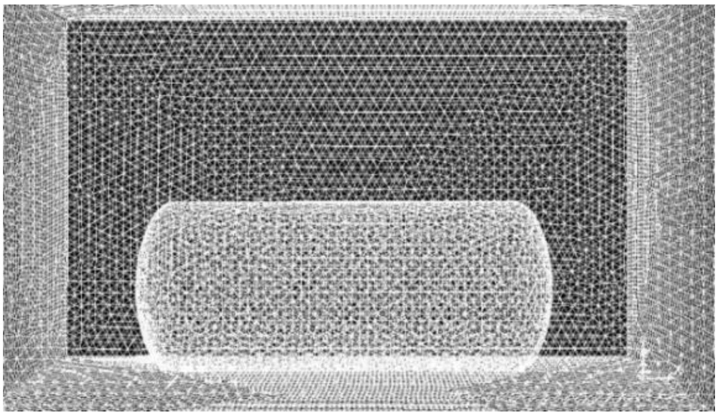


Fig. 4: meshing of the chlorine storage (one million meshes)

approach could suffice. The mesh, made by employing the software GAMBIT, entailed about 1000,000 nodes as displayed in Figure 4.

The simulations related to the spreading gas were executed on an Intel ® Corei7 computer with a characteristic time step size of 10 seconds. Initial spreading calculations with a time step of 1 second were performed and the comparison showed that a step size of 10 seconds would be adequate. It is assumed that isothermal condition dominates during the simulation. The significance of the turbulence intensity in the internal flows can be great with values between 1 to 10% at the inlet. Thus, in this simulation the turbulence intensity was 5% (the indoor environment, the temperature scenario). However, in the wind velocities and the ventilation scenarios, the turbulence intensity was 10%. In case a surface reaction exists, happening on the walls and in case the reaction rate is already identified, it could be simply integrated as a boundary condition. Likewise, if the scalar partakes in a homogeneous chemical reaction along with various constituents of the gas, it might be integrated simply as a source or sink term. Consequently, a reacting gas case can be certainly taken into consideration by the present approach. Yet, a two- (or multi-) phase formulation will be needed in case a phase change such as condensation. In fact, the boundary conditions are in accordance with the case of a dispersion of a non-reacting gaseous scalar.

RESULTS AND DISCUSSIONS

Temperatures

In this section the effects of various temperatures (270K, 297K and 315K respectively) on gas diffusion are considered in the indoor environment with constant amounts of time and the mass flow-rate of the gas (which assumed to be 0.01 $kg.\min^{-1}$ from the pipe crack in all the simulations). According to figures 5 to 7, there is a considerable discrepancy between the dispersion of the gas in the storage at various temperatures; For instance, there is a safe space (free of chlorine) prior to 500 seconds (about 8

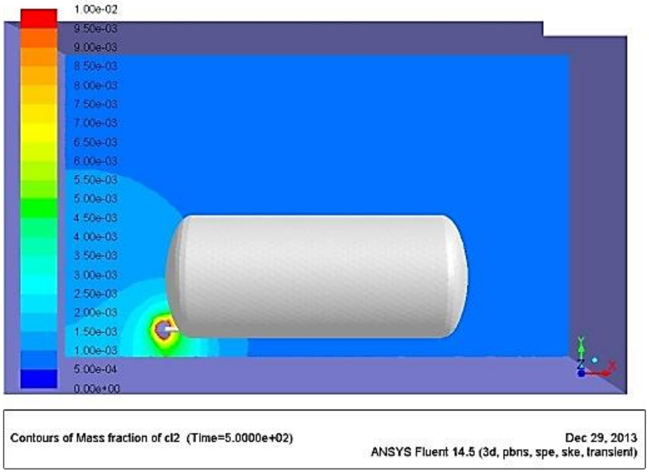


Fig. 5: The mass fraction of cl2 in the indoor environment at 270k in 500 seconds.

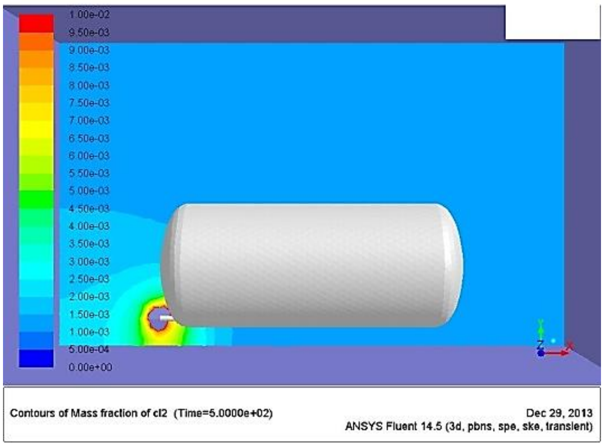


Fig. 6: The mass fraction of cl2 in the indoor environment at 297k in 500 seconds.

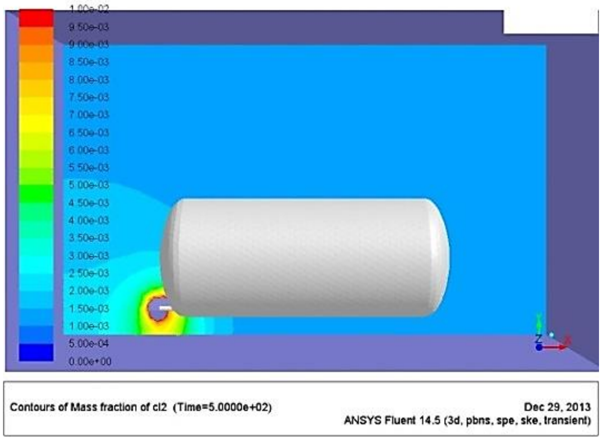


Fig. 7: the mass fraction of chlorine in the indoor environment at 315k in 500 seconds.

min) when the temperature is 270K (Figure 5) the gas diffused $4.50e^{-3}$ while at the same time all space of the room was covered by the gas in the other temperatures (Figure 6 and 7); likewise, at 315K (Figure 7) the diffusion of Cl_2 was faster contrasting the natural temperature. Therefore, there was a direct correlation between the temperature and gas spreading.

Wind Velocities and Same Temperatures

For all the following figures (8-16) the amounts of mass flow-rates assumed to be constant at 0.01 $kg\,\min^{-1}$, but the time considered variable.

Results of Cl_2 leakage at 270K in various wind speeds

One of the most important points in diffusion of heavy gases is the flow direction and the wind velocity in the surrounding environment from the source of the leak. Figure 8 shows the chlorine gas dispersed to the ground level at the flow-rate of 1 $m.s^{-1}$ while it changed its direction towards the top of the tank at 3 $m.s^{-1}$; however at 5 $m.s^{-1}$ there seems to be just a few leaking which can be disregarded, because the wind velocity makes different turbulent flows around the tank, as shown in Figures 8 to 10.

According to the displayed figures, the turbulent flow in Figure 8 is condensed and the flow direction goes to the ground while Figure 9 indicates that the direction of the gas turbulence goes to the top of the tank and the turbulent flow is bigger than the one in the previous figure. On the other hand, Figure 10 displays that the

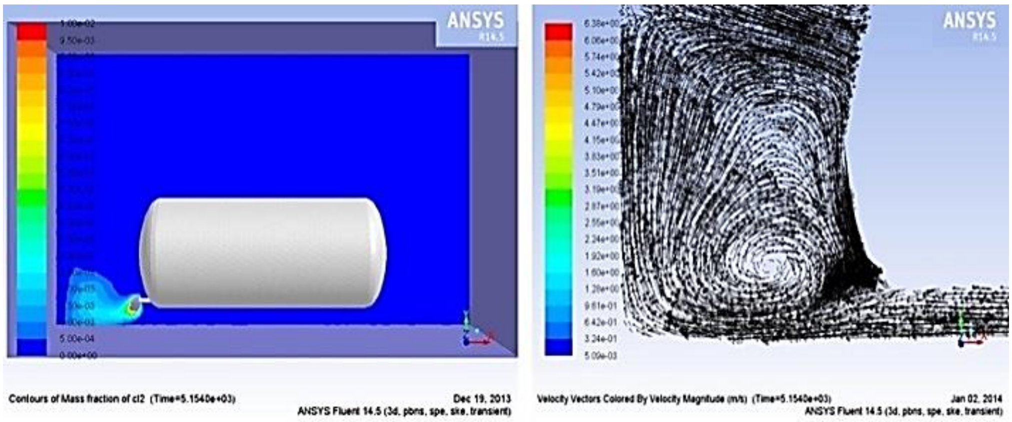


Fig. 8: the velocity vector of cl_2 in the storage at 270k at a 1 $m.s^{-1}$ wind speed

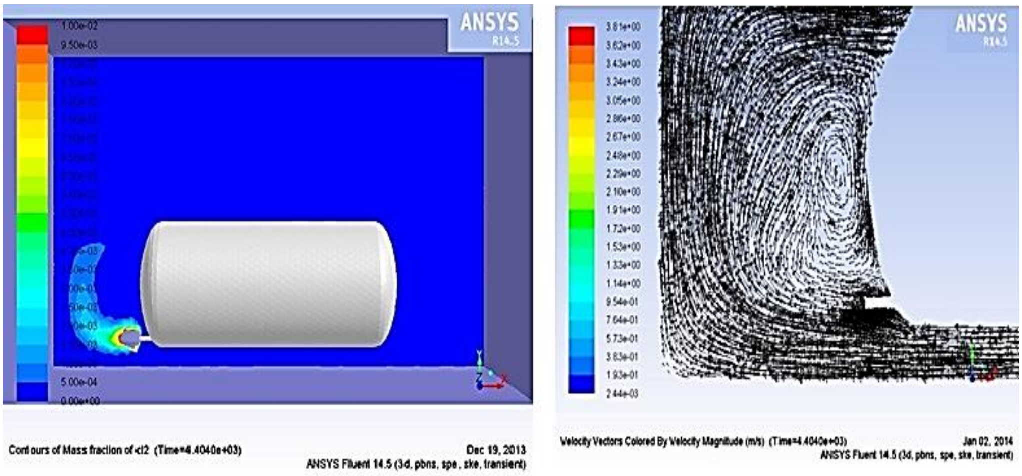


Fig. 9: the velocity vector of cl_2 in the storage at 270k at a 3 $m.s^{-1}$ wind speed

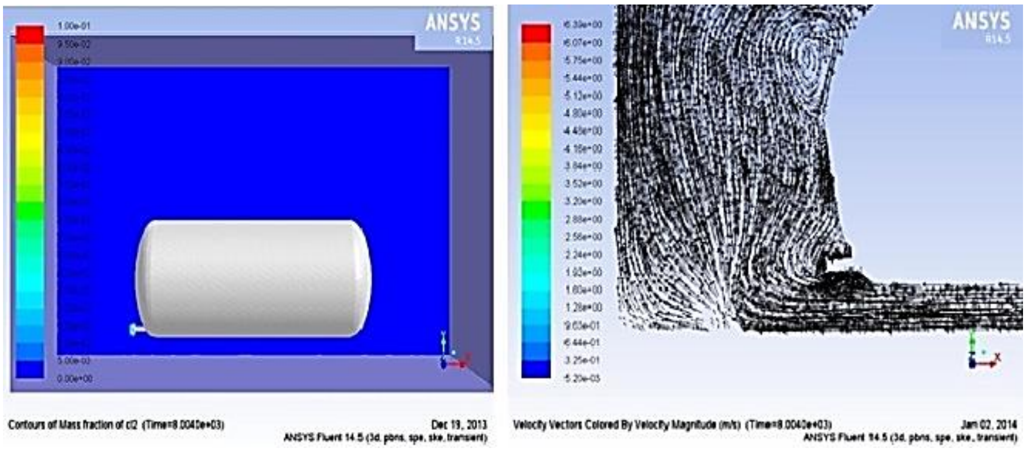


Fig. 10: the velocity vector of cl$_2$ in the storage at 270k at a 5 $m.s^{-1}$ wind speed

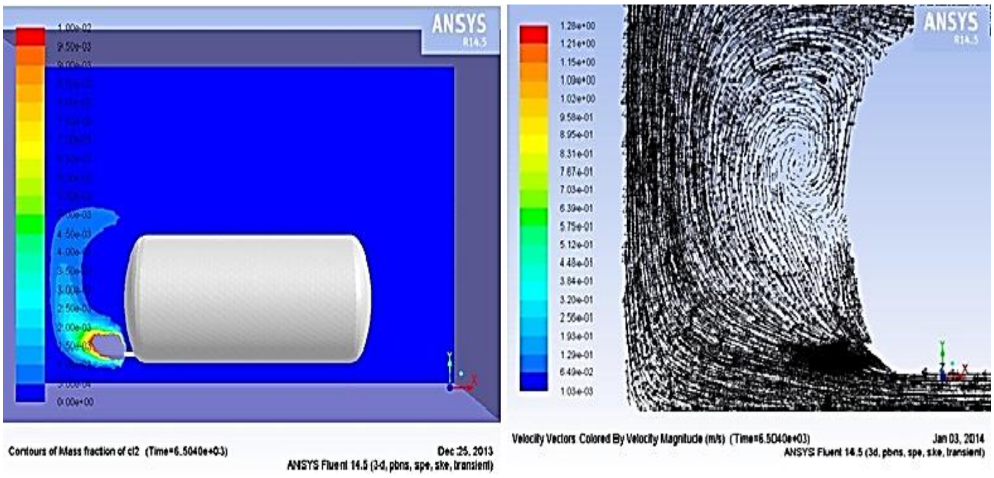


Fig. 11: The mass fraction of cl2 in the indoor environment at 297k in 500 seconds.

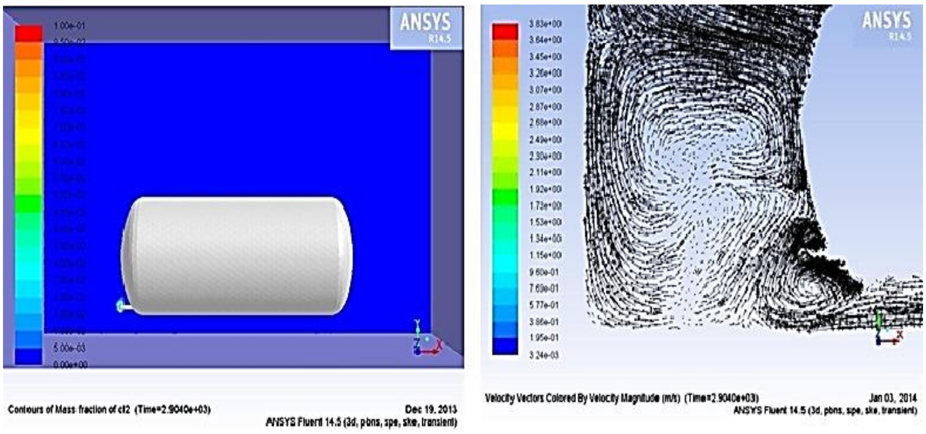
direction of the turbulence in front of the tank is very unequal and the turbulent flow constituted near the leak point is slight.

Results of the Cl$_2$ release at 297K in various wind velocities

As indicated in Figure11, there is a constant and great turbulent flow in front of the leak source while the actuated gas to the top of the tank is also very regular and its direction prevented the heavy gas from going to the ground level. In Figure 12, it is seen that there are three turbulent flows around the leak point that affected each other and kept the gas near the tank while preventing the chlorine spread in the storage. Finally, the wind speed in Figure 13 is shown to cause a very strong and regular turbulent current in front of the tank affecting the gas diffusion in the environment; consequently, Cl$_2$ was held around the ground level while its dispersion in the storage is prevented.

Investigating the results of Chlorine leakage at 315K in various wind speeds

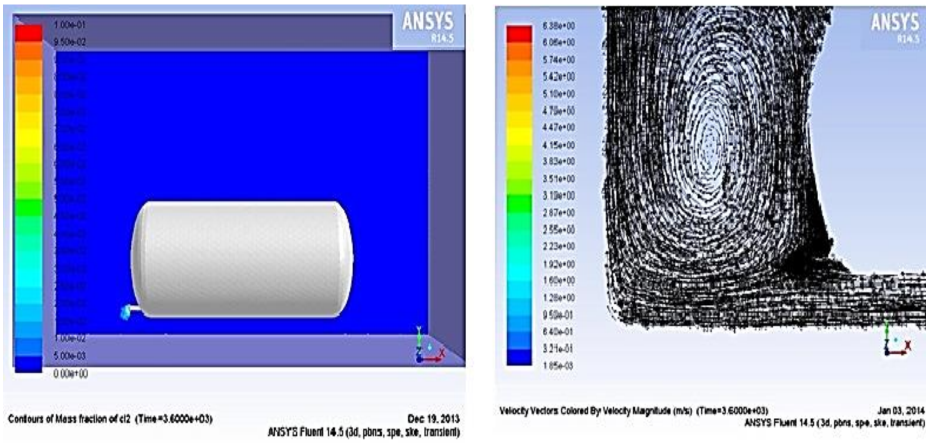
In Figure 14, it can be discerned that there was no turbulent flow in front of the tank; furthermore, according to the contour pictures, chlorine spread from the space near the wall because the wind directions were formed there; while there is a great turbulent flow near the leak point at a $3\,m.s^{-1}$, this flow along with the direction of the wind caused the Cl_2 being kept around the ground level, as exhibited in Figure 16. When the amount of the wind speed rose to $5\,m.s^{-1}$, the direction of the chlorine dispersion changed toward



Contours of Mass fraction of cl2 (Time=2.9040e+03) Dec 19, 2013
ANSYS Fluent 14.5 (3d, pbns, spe, ske, transient)

Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=2.9040e+03) Jan 03, 2014
ANSYS Fluent 14.5 (3d, pbns, spe, ske, transient)

Fig. 12: The velocity vector of cl_2 in the indoor environment at 297k at a $3\,m.s^{-1}$ wind speed



Contours of Mass fraction of cl2 (Time=3.6000e+03) Dec 19, 2013
ANSYS Fluent 14.5 (3d, pbns, spe, ske, transient)

Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=3.6000e+03) Jan 03, 2014
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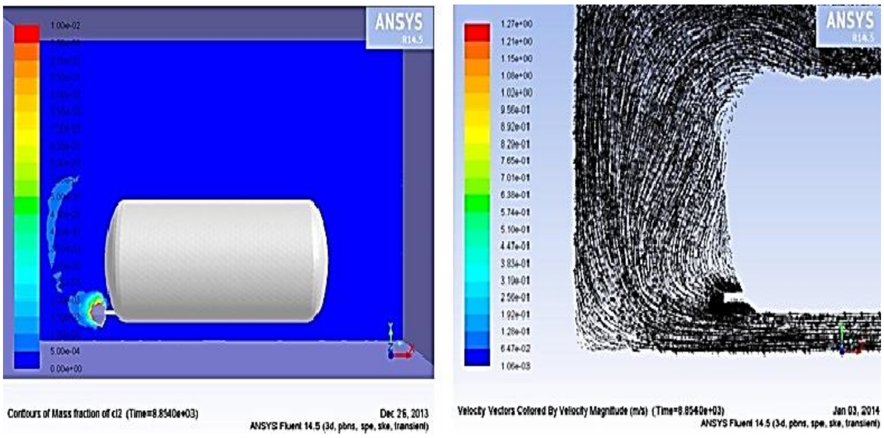
Fig. 13: The velocity vector of cl_2 in the indoor environment at 297k at a $5\,m.s^{-1}$ wind speed



Contours of Mass fraction of cl2 (Time=8.8540e+03) Dec 26, 2013
ANSYS Fluent 14.5 (3d, pbns, spe, ske, transient)

Velocity Vectors Colored By Velocity Magnitude (m/s) (Time=8.8540e+03) Jan 03, 2014
ANSYS Fluent 14.5 (3d, pbns, spe, ske, transient)

Fig. 14: the velocity vector of cl_2 in the storage at 315k at a $1\,m.s^{-1}$ wind speed

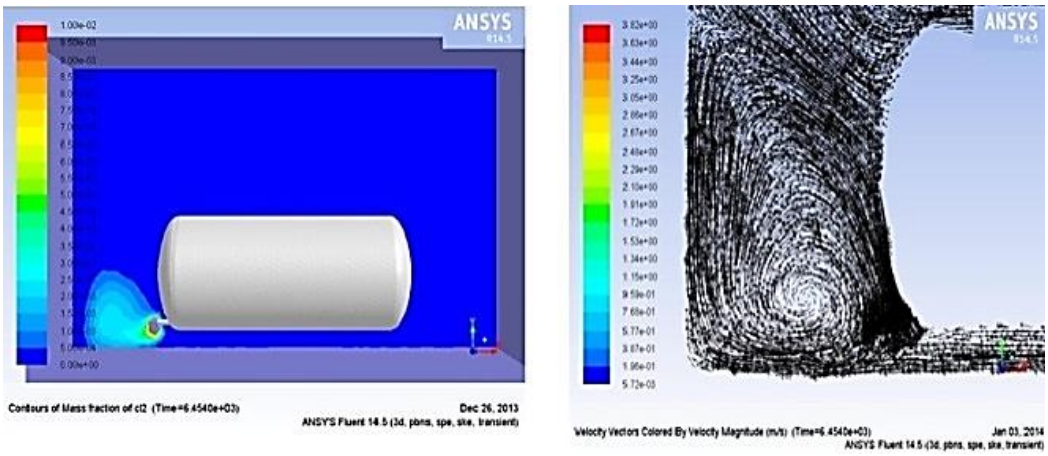


Fig. 15: The velocity vector of cl$_2$ in the storage at 315k at a 3 $m.s^{-1}$ wind speed

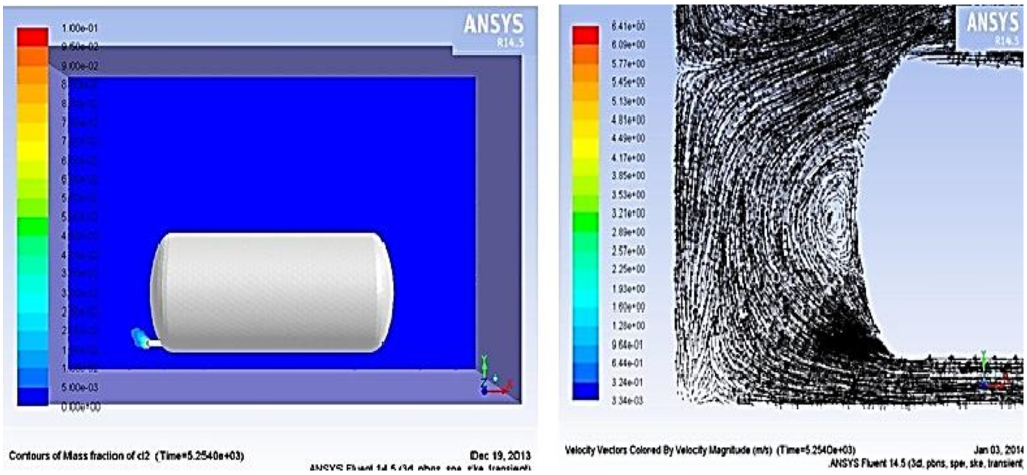


Fig. 16: The velocity vector of cl$_2$ in the storage at 315k at a 5 $m.s^{-1}$ wind speed

the top but the turbulent currents prevented the gas from spreading to the top of the tank. The important point is that the higher speed caused a reduction in the concentration of the heavy gas in the environment.

Ventilation

The effects of the air flow is made by ventilation on the chlorine dispersion in the storage are shown in Figure 17. Some turbulent currents are made in front and top of the tanks directly affecting the spread of the heavy gas in the room. The turbulent flows near the leak point and the front of the ingress ventilation are exceedingly strong because in these parts the gas outlets from the tank and the air entrance changed the direction of the air current, as displayed in Figures 17 and 18.

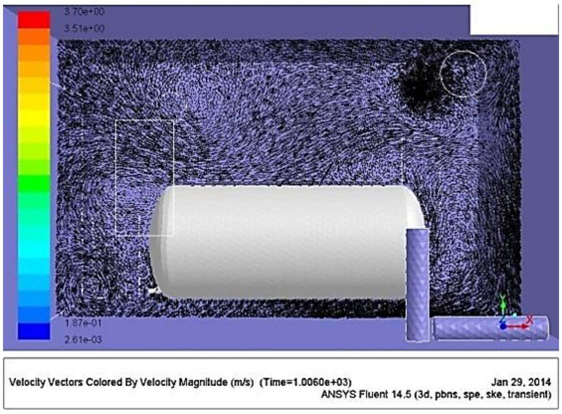


Fig. 17: The velocity vector of Cl$_2$ in the storage with the ventilation

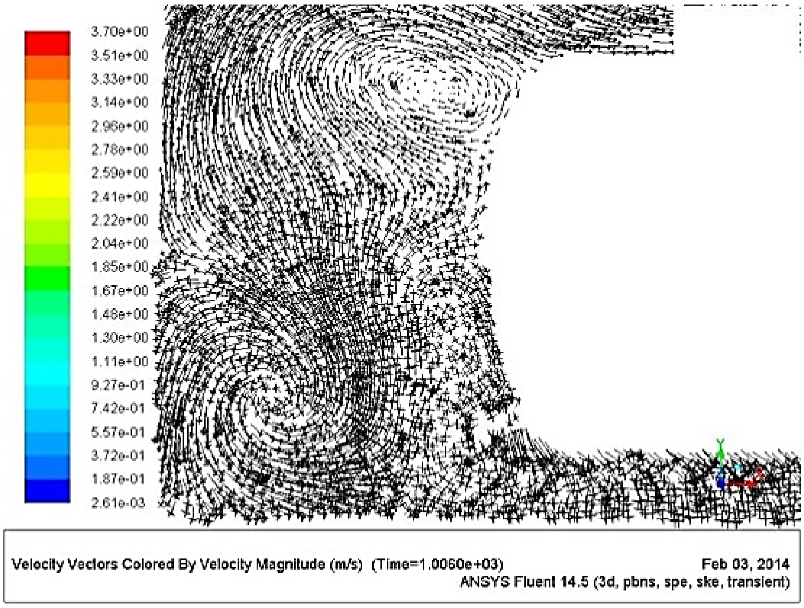


Fig. 18: The velocity vector of Cl_2 direction in front of the chlorine tank

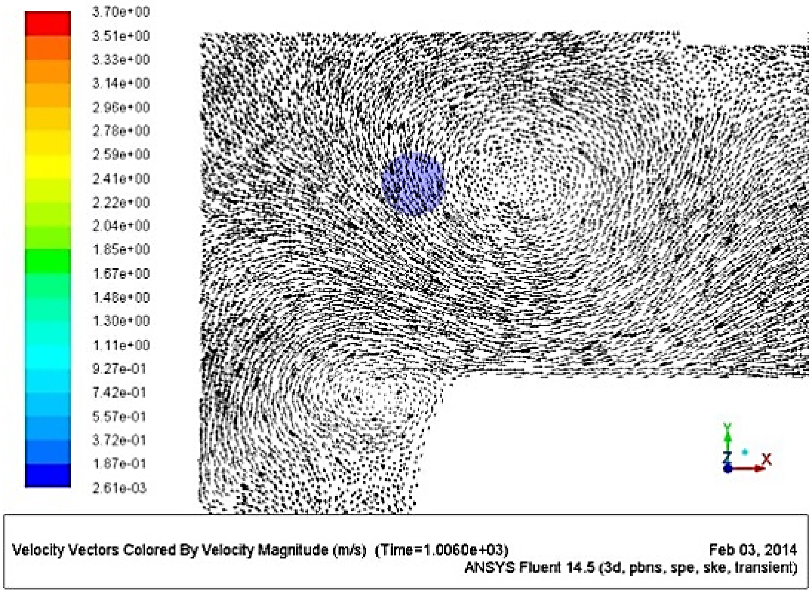


Fig. 19: The velocity vector of Cl_2 direction in front of the outlet ventilation

According to Figure 18, the turbulent flow direction caused the chlorine gas to move toward the top of the tank; On the other hand, the exhaust ventilation sucked the air strongly and conducted the mixture of chlorine and the air toward outside of the storage which is shown in Figure 19. In addition, the turbulent flow is made by the inlet ventilation to prevent the dispersion of the heavy gas in the back and beneath of the tank and led the air to outlet ventilation which is depicted in Figure 18. In other words, the directions of the turbulent current are made by the inlet and outlet ventilations and the chlorine leakage had direct effects on the chlorine spread in the room. Consequently, most of the space is safe for the workers when the ventilation is functioning; for instance, the space behind of the tank is safe.

CONCLUSIONS

In conclusion, the results from the simulations revealed that the heavy gas spread like a liquid and it stayed near the ground floor when there were no wind velocities in the environment or the wind speed was very slow. Furthermore, this research indicated that there were direct relationships between the changes made on the temperature and the diffusion of the heavy gas in the environment. In other words, when the temperature goes up in the indoor environment, the diffusion speed of the chlorine in the air rises dramatically. Also, the effects of the wind velocity were investigated in this research proving that the wind speed could change the direction of the dispersion as well as preventing the Cl_2 spread in the space. In other words, the simulations indicated that the dilution, wind velocities, and the direction of the turbulent flows could directly affect the dense gas dispersion.

There is a direct relationship between the diffusion of denser chlorine in the air and the ventilation performance. The ventilation leads the chlorine mixture and the air toward outside as well as preventing gas spread in the room. Therefore, the best system for keeping the space safe and reducing the cost of the damages is suitable ventilation.

REFERENCES

1. Anonymous, *Chlorine Safe Work Practices*. Compensation, Workers Columbia, British, 2006, pp. 1–44.
2. C. Winder, "The toxicology of chlorine.," *Environ. Res.*, vol. 85, no. 2, pp. 105–14, Feb. 2001.
3. J. García, E. Migoya, J. a Lana, and a Crespo, "Study of the dispersion of natural gas issuing from compressor stations through silencers with upper cover.," *J. Hazard. Mater.*, vol. 152, no. 3, pp. 1060–72, Apr. 2008.
4. M. Kiša and Ľ. Jelemenský, "CFD dispersion modelling for emergency preparadnes," *J. Loss Prev. Process Ind.*, vol. 22, no. 1, pp. 97–104, Jan. 2009.
5. M. Pontiggia, G. Landucci, V. Busini, M. Derudi, M. Alba, M. Scaioni, S. Bonvicini, V. Cozzani, and R. Rota, "CFD model simulation of LPG dispersion in urban areas," *Atmos. Environ.*, vol. 45, no. 24, pp. 3913–3923, Aug. 2011.
6. M. Siddiqui, S. Jayanti, and T. Swaminathan, "CFD analysis of dense gas dispersion in indoor environment for risk assessment and risk mitigation.," *J. Hazard. Mater.*, vol. 209–210, pp. 177–85, Mar. 2012.
7. P. Gilham, S., Deaves, D. M., & Woodburn, "Mitigation of dense gas releases within buildings: validation of CFD modelling.," *J. Hazard. Mater.*, vol. 71, no. 1–3, pp. 193–218, Jan. 2000.
8. P. Schmittinger, *Chlorine–Principles and Industrial Practice*. Weinheim, Germany, 2000, pp. 159–222.
9. R. Pontiggia, M., Derudi, M., Busini, V., & Rota, "Hazardous gas dispersion: a CFD model accounting for atmospheric stability classes.," *J. Hazard. Mater.*, vol. 171, no. 1–3, pp. 739–47, Nov. 2009.
10. S. Cheng, G. Chen, Q. Chen, and X. Xiao, "Research on 3D dynamic visualization simulation system of toxic gas diffusion based on virtual reality

technology," *Process Saf. Environ. Prot.*, vol. 87, no. 3, pp. 175–183, May 2009.

11. S. Gilham, D. Deaves, and R. Hoxey, "Gas build-up within a single building volume—comparison of measurements with both CFD and simple zone modelling," *J. Hazard*, vol. 53, no. 1, pp. 93–114, 1997.