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Chlorine Gas Releases in Urban Area: Calculation of Consequences through CFD Modeling and Comparison with Standard Software

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This paper focuses attention on emergency management associated a chlorine gas release in urban area. In particular we want to show how the complexity of the geometry of a city could affect the distribution of a cloud of toxic substance. For this reason, it was simulated by the CFD code Fluent a release of chlorine and has compared the result with a simulation carried out with standard code for risk analysis, in our case PHAST.

1. Introduction

The study of release of hazardous substance is characteristic of risk analysis. The release may be caused by accident event involving plant or material transported by roadway and railway. Substances transported by road or train can produce effects greater than for plant installations, because the location of these substances can pass through the high population density areas as in the urban centre. the past few years, after the attack of the twin towers, the substances transported by road are used in terrorist attacks in sensitive areas like the center of a city (Lisi R., et al, 2007; Maschio G., Milazzo M.F., 2008)

The gas release is characterized by the degree of atmospheric turbulence. This parameter affects the mixing of cloud with the surrounding air. The atmosphere turbulence is caused by friction between the ground and air. So the parameter that characterizes the turbulence and therefore the dispersion is the ground roughness. Ground roughness is determined by number and size of roughness elements present in an area. In conventional codes for the study of risk analysis, such as PHAST (DNV Software), the ground roughness makes homogeneous the ground, and the code don't consider the contribution of the singular parts that constituent the ground. The study area appears to plane geometry or two-dimensional.

In the case of urban areas and thus made complex by the presence of many buildings, the gas dispersion is affected, there may be channels or points of stagnation gas.

For this reason we studied a release of chlorine in three-dimensional urban environment with code CDF Fluent (Scargiali F. et al, 2008; Di Sabatino et al, 2008)

In particular we studied a release of chlorine gas. This substance is widespread and used; for this reason transport of chlorine by road or rail is common. In fact, chlorine is one of the toxic substances used for terrorist attacks.

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Chlorine is a toxic gas and is transported under pressure. The release of this substance will produce a two phases jet from which causes a cloud of heavy gas (High molecular weight 70.09 kg/kmol).
A release of toxic substances in the environment can cause harm to exposed individuals ranging from irritation, a non-fatal injuries to death. To properly assess the effects of exposure you may need to know a relation that links the profile of concentration of toxic substance in time with the level of damage suffered by the individual exposed. For chlorine can be exposed without health consequences to the concentration of 1 ppm for 10 minutes or at a concentration of 0.5 ppm for 60 minutes. On the contrary, is fatal in 50% of cases, exposure to 20 ppm for several hours, to 33 ppm for one hour or 60 ppm for 10 minutes. For this study was taken as the limit value "Immediately Dangerous to Life or Health" (IDLH), and is defined by the US National Institute for Occupational Safety and Health (NIOSH). This parameter for chlorine is equal to 25 ppm.
In the following section, shows procedures and simulations carried out with CFD code Fleunt, and standard code of risk analysis Phast.

2. Geometry

The geometry chosen for the simulation concerns a real district but anonymous town, which are openly available online data on the geometry, and plant height of buildings, and the data of a simulation conducted in tunnel wind for that geometry. This will then carry out a simulation of a real complex urban area and has the opportunity to compare the results with reliable experimental data.
The geometry chosen for the simulation, shows in figure 2.1

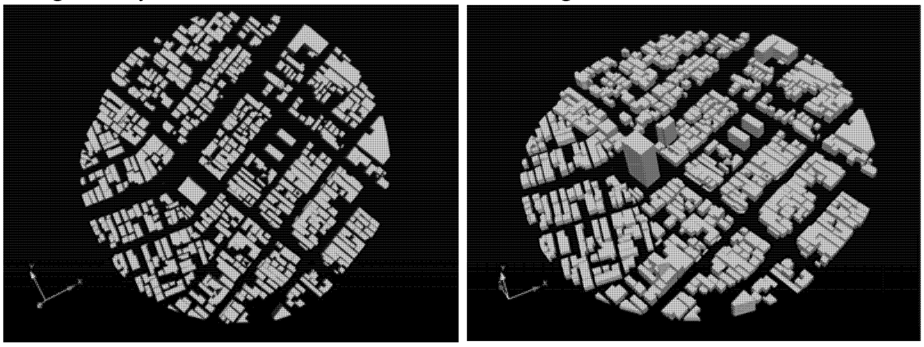


Figure 2.1 Map of area

For the construction of the domain and the creation of the mesh we followed the tutorial *Gambit tutorial 03 – Simulation of wind around buildings*.

3. Fluent Simulation

Fluent allows to see the evolution of the dispersion of the toxic over time. This is achieved by setting up a dynamic simulation is divided into three main steps, which summarize the evolution of the toxic cloud from its generation to its transport in the domain.

STEP 1: we make a first simulation to obtain the stationary wind profile, is done by setting the boundary conditions in the entrance wall of the toxic substance as to have no entry of the substance. It then solves the system in the sole presence of air and wind profiles are generated as before in the study of fluid dynamics of the system. The file generated by the convergence of this first step is used as the initial condition at time zero of the next step of the problem. For this step we followed the tutorial *Fluent tutorial 03- Simulation of wind around building* (Russell A., 2009). The convergence of the simulation is accomplished by setting the k-ε model. The under relaxation factors used are 0.1 to 0.3 for pressure and momentum. We also used a model of type SIMPLE. Finally, we used a discretization of second order.
In figure 3.1 shows the velocity vectors to the plan with particular interest in the road near the highest building where the first entry of the pollutant.

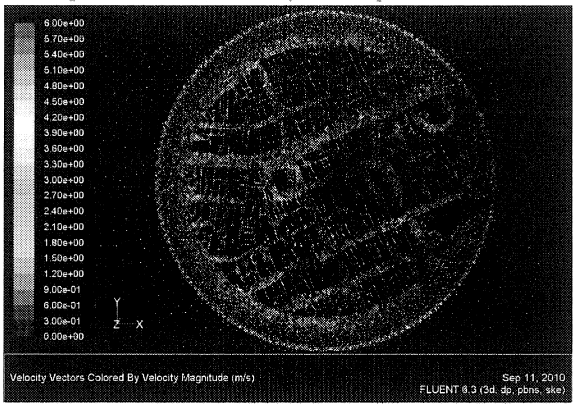
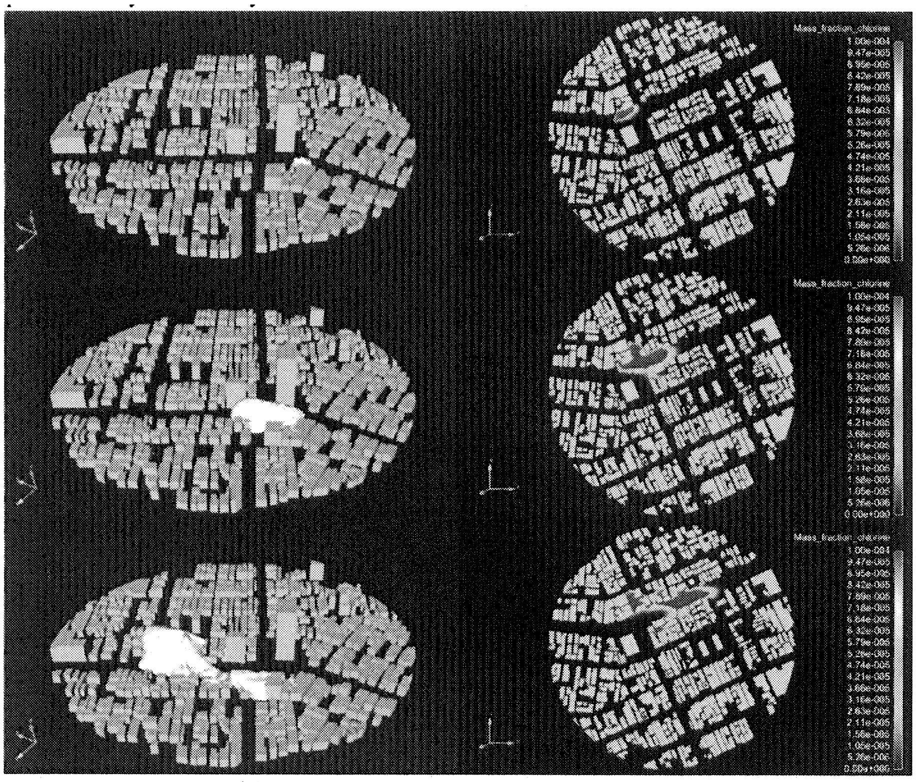


Figure 3.1 Velocity vector to the plan seat height of two meters above the ground

STEP 2: the initial conditions are those of the previous step. It will then perform a second simulation of non-stationary dispersion by changing the entrance *wall* to the *mass flow inlet* for entry of chlorine. In the simulation will be set to the equation of transport of chemical species without reaction so you can then retrieve the results in terms of concentration of the toxic substance in the system. It will also set the time step and the maximum number of time steps to simulate that coincides with the time of issuance of the toxic environment. We can save the results and images on each time step x, consult the guide Fluent in the section on simulations where the time dependence is well explained how to set a non stationary case and how to save the simulation results. At the end of the time intervals you can then get a series of simulations in which time saved in the cloud is generated and at the same time moves in the domain. The file saved at the last time step will be used as an initial condition of the next step. The approaches adopted for the simulation are the same of STEP1

STEP 3: we make a final simulation to see how the cloud is generated in the previous step, moving along the domain. The initial conditions of this simulation are not stationary for the last time step of the previous case for which you must read file for that step. The entry of the toxic substance will again be a *mass flow inlet* to *wall* and the simulation will take place during a different non-stationary time series of steps for a total time corresponding to the time of our interest, possibly to the exit of the cloud from the domain or the dispersion of the toxic concentrations to values low enough to no be dangerous. Again you can save a series of images and results during the simulation to see how the cloud moves in the domain.

You choose to impose an inflow of chlorine of 1.5 kg/s for a total of 20 seconds (STEP 2). Then you set a shift of the cloud generated along the domain of a further 60 seconds (step 3). The results generated in 3D by setting an iso-surface with a value of IDLH are shown in Figure 3.2(a). In Figure 3.2(b) we report the concentration profiles of the cloud on a flat place to two meters above the ground versus time; IDLH value is represented by the color yellow.



(a) *(b)*

Figure 3.2 Sequence of images related to the displacement of an isosurface with a value equal IDLH chlorine concentration: (a) 3D vision, (b)two-dimensional plane.

4. Standard Software Simulation

Phast (Process Hazard Analysis Software Tool) programmed by DNV Software. The software is a comprehensive consequence analysis tool. It examines the process of a potential incident from the initial release to its evolution such as dispersion, including modeling of pool evaporation, and flammable and toxic effects.

The simulation of the release of chlorine was carried out with the same inputs of the simulation carried out with Fluent. In particular, the source is defined as a release of chlorine in the liquid phase. The release is characterized by a flow rate of 1.5 kg/s for a duration of 20 seconds. The weather conditions included are:wind speed at the source of 3 m/s; temperature of 10 ° C and relative humidity of 70%.
A key parameter to define the release is the surface roughness in this case is 3 m as the area is the center of a city characterized by buildings.The results obtained are a cloud of chlorine as a function of concentration and time of release.

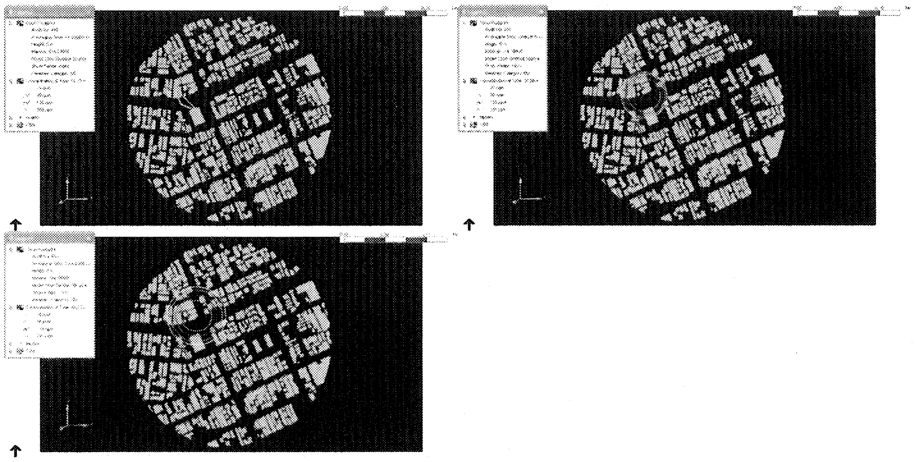
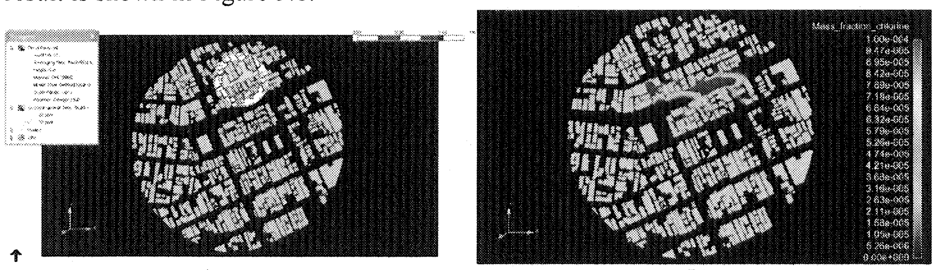


Figura 4.1 A sequence of images on the simulation code by Phast. The yellow area shows the relative concentration of IDLH.

5. Conclusion

It is now interesting to study the shape of the cloud at the end of the simulation. As for the code Phast, which is not affected by the presence of buildings, the cloud has moved in the direction and speed data from the assigned settings. In practice, the cloud moves as if the domain is empty and does not take into account the presence of obstacles. This result is shown in Figure 5.1.



(a) *(b)*

Figure 5.1 Comparison of the impact areas of the cloud after 80 seconds of simulatio: (a)PHAST, (b) Fluent.

Completely different is the shape of the cloud generated by the software Fluent. The cloud is influenced into account the presence of buildings; and are created zones where the funnel faster wind carries the cloud. In addition to these areas of higher speed are also areas of stagnation due to the presence of buildings in these areas: can be observed that the cloud remains trapped for more time. The impact zones are therefore very different and so are the times of extinction of the cloud.
We want to point out that the simulation with Fluent is laborious and time consuming. Furthermore, it is always advisable to compare with experimental data in the wind tunnel to verify that the fluid solution is accurate.
It is therefore appropriate to use the CFD code to simulate an accident or a terrorist attack, especially when dealing with sensitive targets. In all other cases, such as an emergency measure, it is preferable to an approximate solution created using standard code that returns the required results in minutes. In the case of a toxic substance, to make the results more conservative values it is better to use a concentration of 1 / 10 of IDLH.

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