CHLORINE GAS RELEASES IN URBAN AREA: CALCULATION OF CONSEQUENCES THROUGH CFD MODELING AND COMPARISON WITH STANDARD SOFTWARE

Chiara Vianello, Paolo Albanese and Giuseppe Maschio*

DIPIC - Dipartimento di Principi e Impianti Chimici di Ingegneria Chimica
Università di Padova Via Marzolo, 9 - 35131 Padova
giuseppe.maschio@unipd.it

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, a release of chlorine was simulated by the CFD code Fluent and the result has compared with a simulation carried out with standard code for risk assessment (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. Dangerous goods 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 terroristic attack of the twin towers, the substances transported by road has been used in terrorist attacks in sensitive areas like the center of a city (Lisi R., et al, 2007; Maschio G., Milazzo M.F., 2008). This fact increase the importance of the investigation of release in urban areas.

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 consequences, 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 the following section, shows procedures and simulations carried out with CFD code FLUENT, and standard code of risk analysis PHAST.

2. CHLORINE

Chlorine is a very toxic gas usually transported under pressure. This substance is widespread and used; for this reason transport of chlorine by road or rail is common. In addition chlorine is one of the toxic substances more utilized in recent terrorist attacks.

The release of this substance should be described in two step from a jet release of under pressure gas which causes a cloud of heavy gas after the dispersion in the atmosphere. In table 1, shows the physical property of chlorine.

Table 1 Physical property of chlorine

Property	Value
Molecular weight (g/mol)	71
Boiling point	- 34 °C
Melting point	- 101 °C
Critical temperature	144 °C
Density (air=1)	2.5
Liquid density	1.6
Vapor pressure (20 °C)	6.8 bar
Solubility in water (mg/l)	8620
Physical description	Greenish-yellows gas
Odor	Pungent
Autoignition temperature	NA
Flammability limits (vol % in air)	NA

2.1. Toxicity data

A significant release of toxic substances in the environment can cause different degrees of damage due to exposed individuals such as irritation, non-fatal injuries or 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 example, the following table shows the dose / effect relationship for acute exposure to chlorine inhalation.

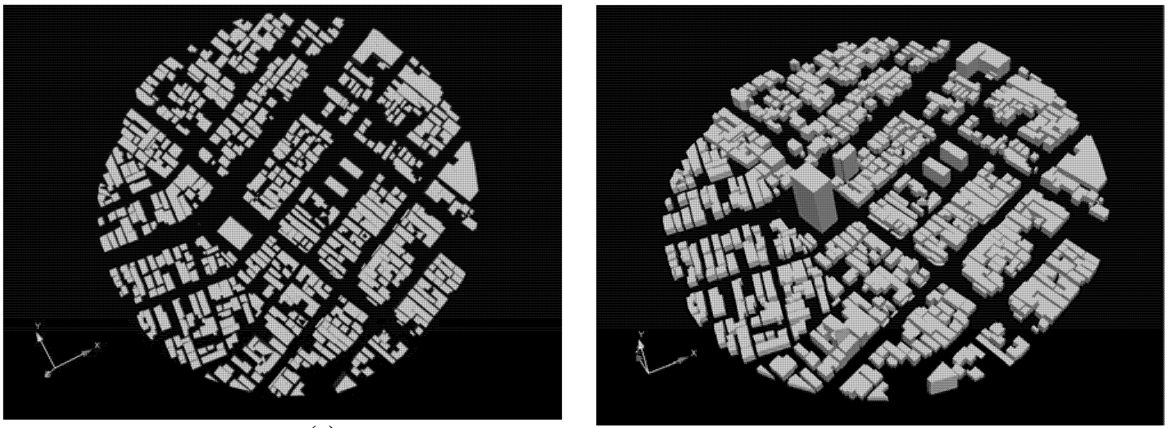
Table 2. Tipical value of concentration for relationship dose/effect of chlorine

Concentration in air (ppm)	Effect on exposed individual
0.2-0.5	Odor threshold
0.5	TLV – TWA
1	TLV – STELL
1.3	Severe respiratory failure after 30 min
3.5	Perceptible in air
>5	Severe irritation of skin and mucous membrane in few minutes
14-21	Danger after 30-60 min
25	IDLH
40-60	Toxic pneumonia and pulmonary edema
430	Lethal for exposition upper 30 minutes
1000	Lethal in few 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.

3. URBAN AREA

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 was developed by Autocad: starting from the plant were extruded all the buildings to their height. The buildings were represented as parallelepipeds and the geometry is exactly identical to that simulated in the wind tunnel.
The geometry chosen for the simulation, is show in figure 1



(a)
(b)
Figure 1 Map of area: (a)2D plane, (b)3D

For the starting point of the dispersion of chlorine, we choose to insert a square face of a size equal to 2x2 m^2. This face is inserted near the highest building.
The geometry was imported into the Gambit software to create the mash, and set the boundary conditions

3.1. Mesh and boundary conditions

The creation of the mesh was made following steps:

- Creation of the grid for the base of the buildings containing sub-domain. Because of the special geometry we choose a grid with triangular elements by size function to curb the buildings using a schema type Pave.
- Creation of the grid for the volume containing the buildings, we choose to create a mesh-type TGrid as it adapts easily to different types of geometry. Before creating the mesh of the volume should be established that the face side of the cylinder by means of quadrilaterals and a schema map.
- Then we create the mesh on the lower volume of the remaining domain. After creating the grid on the bottom base, curb and into the cylinder composed of quadrilaterals arranged using a schema Pave, thus creating the volume mesh using a schema TGrid. Even in this case you should create the grid of the lateral surfaces in the same way as the volume containing the buildings.
- Finally, we create the grid of the two remaining volumes by way of a scheme Cooper, the side faces of both volumes may be thickened to the domains so that lower to the upper surface of the domain there are fewer of cells.

The result of proceeding is show in figure 2.

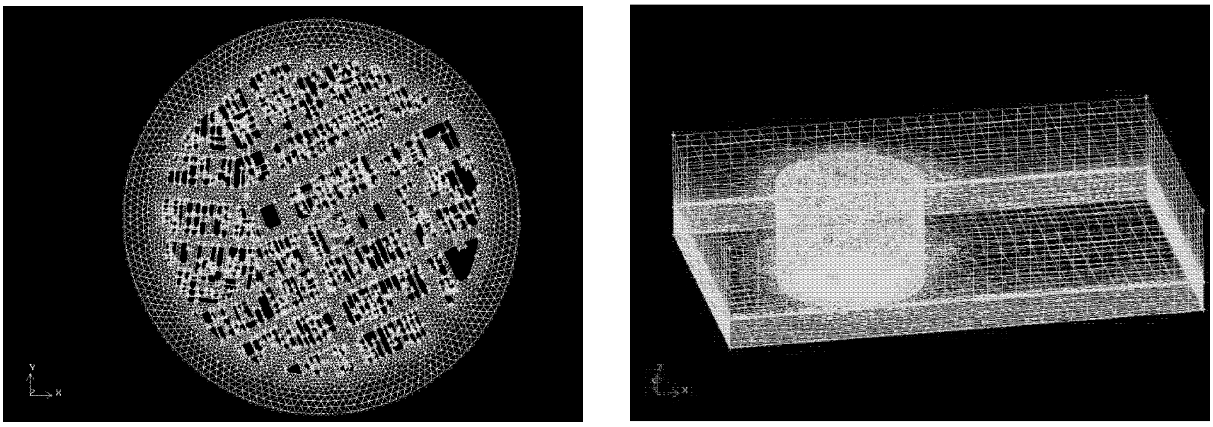


Figure 2 Computational domain and grid

The boundary conditions, to be set in software GAMBIT, are listed below:

- On the surface soil and building facades set as *wall;*
- Side and top surfaces of the domain set as *symmetry;*
- Surface wind input set as the *velocity inlet;*
- Emitting surface of the domain set as the *pressure outlet.*

4. SIMULATION WITH CFD - FLUENT

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 (P. Albanese, 2010).

STEP 1: a first simulation is used 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 STEP1.dat 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.

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.

STEP 3: you 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.

4.1. Fluid dynamic (STEP 1)

Led to convergence, the software can display the results in three dimensions on whatever plan you want. The results of wind tunnel are shown on a plan to two meters above the ground and normalized with respect to the speed input to the system height of 15.9 meters, height at which they are willing real anemometers. In order to compare the results obtained in this direction are normalized with respect to the input speed of 15.9 meters height, speed which is equal to 4.25 m/s. Figure 3 show the velocity vectors to the plan with particular interest in the road near the highest building where the first entry of the pollutant.

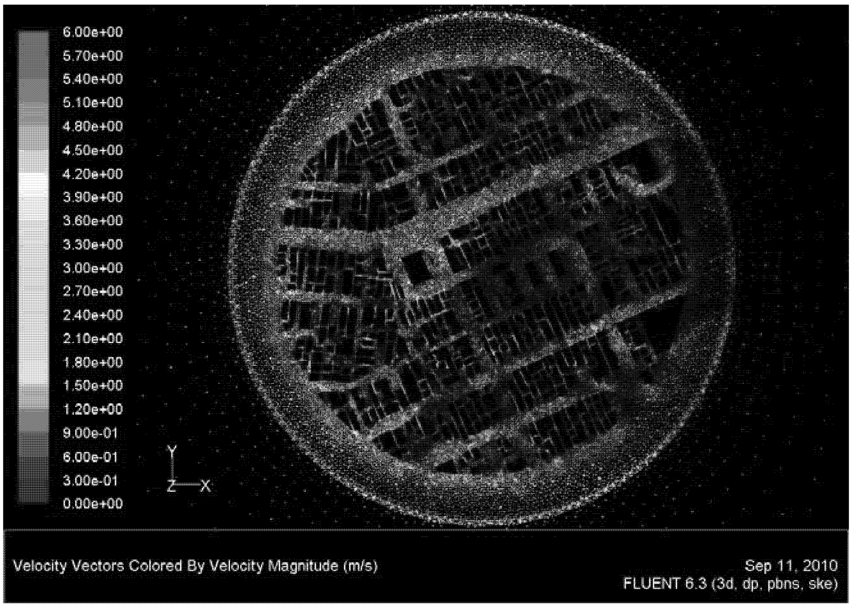


Figure 3 Velocity vector to the plan seat height of two meters above the ground

4.2. Dispersion and propagation (STEP 2-3)

The simulation of the cloud of chlorine is again carried out dynamically. The model of turbulence in this case is as mentioned above the standard k-ε.

The release dispersion was simulated by an inflow of chlorine of 1.5 kg/s for a total of 20 seconds (STEP 2). Then the shift of the cloud generated along the domain of a further 60 seconds (step 3). Figure 4 show the results generated in 3D by setting an iso-surface with a value of IDLH. Figure 5 show the concentration profiles of the cloud on a flat place to two meters above the ground versus time; IDLH value is represented by the yellow area.

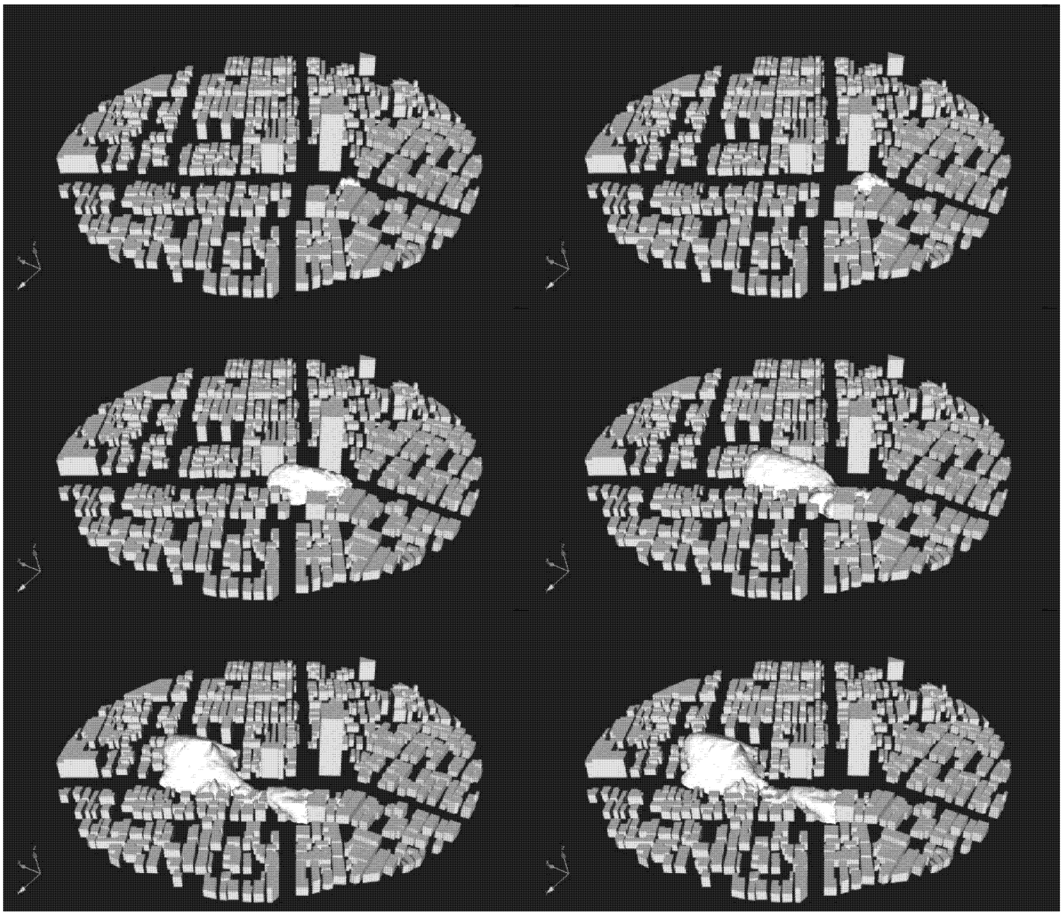


Figure 4. Sequence of images related to the displacement of an iso-surface with a value equal IDLH chlorine concentration.

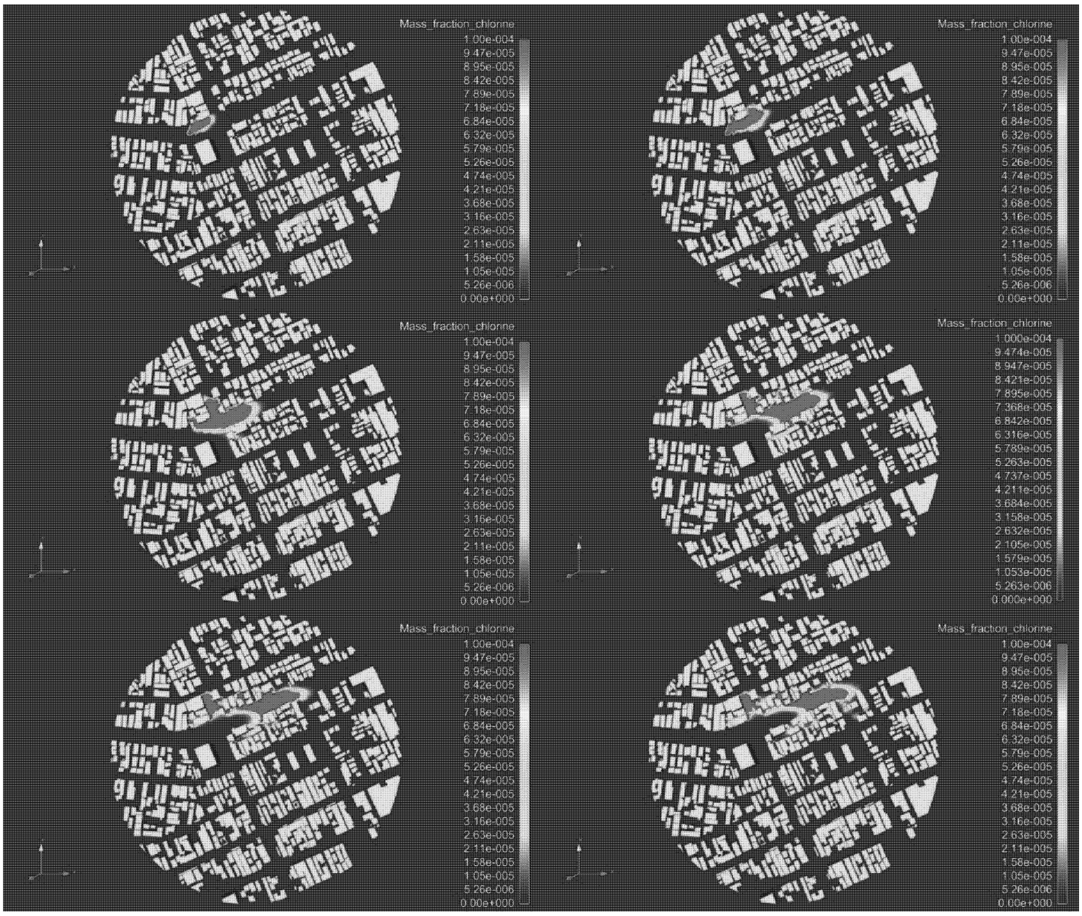


Figura 5. Sequence of images related to the concentration profiles of chlorine and the movement of the cloud during the 80 seconds of simulation.

5. SIMULATION WITH PHAST

The PHAST (Process Hazard Analysis Software Tool) code programmed by DNV Software has been chose for a comparison with the CFD results. 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. PHAST is able to simulate various release scenarios such as leaks, line ruptures, long pipeline releases and tank roof collapse in pressurized or unpressurised vessels.

PHAST has an integral-type dispersion model called UDM [7], Unified Dispersion Model, the model calculates several consequence results: *i)* cloud behaviour; *ii)* transition through various stages such as jet phase, heavy phase, transition phase and passive dispersion phase; *iii)* distance to hazardous concentration of interest and *iv)* trace of the cloud at a given time.

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;
- Relative humidity of 70%;

A key parameter to define the release is the surface roughness. This parameter, expressed in meters, characterizes the type of terrain where there is the release. Typical values of this parameter according to the type of land have already been reported in Table 2.3.

Table 2.3 Typical value of surface roughness in function of type of land

Type of land	**z_0 (mm)**
Completely smooth, ice	0.01
Offshore, calm sea	0.20
Rough sea	0.50
Snow surface	3.00
Grass	8.00
Grassland	10.00
Fallow fields	30.00
Farmland	50.00
Some trees	100.00
Many trees, some building	250.00
Forests	500.00
Suburban	1500.00
Centre of city with tall building	3000.00

For the case considered the surface roughness is 3000 mm 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. Figure 6 shows the evolution of the chorine cloud during the time. The yellow line is representative of the IDLH concentration.

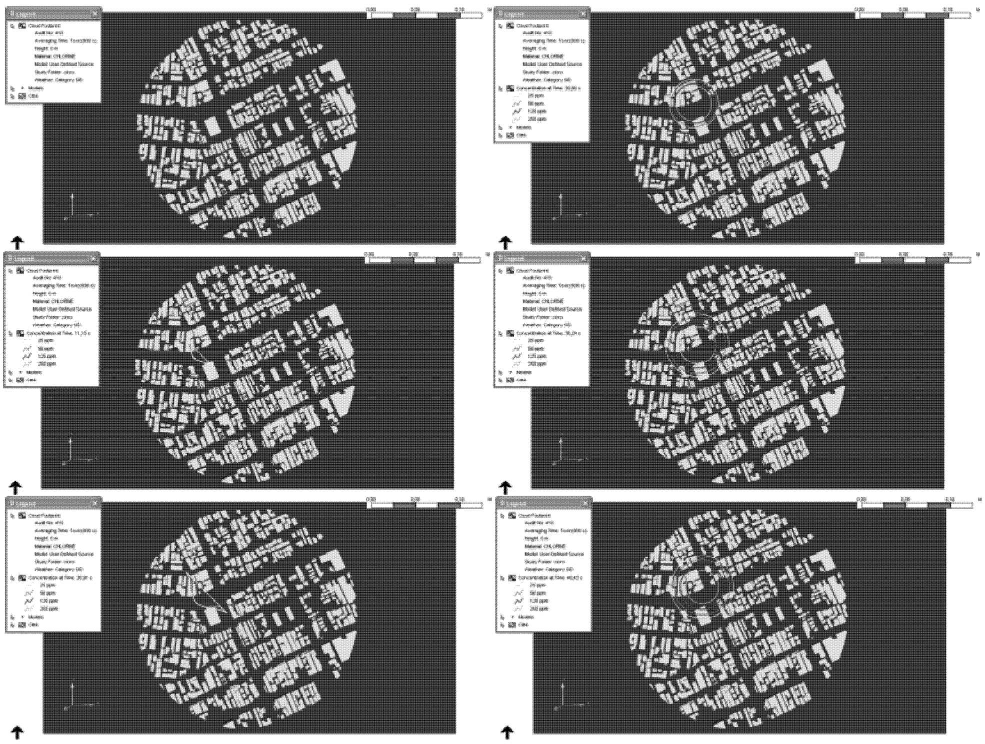
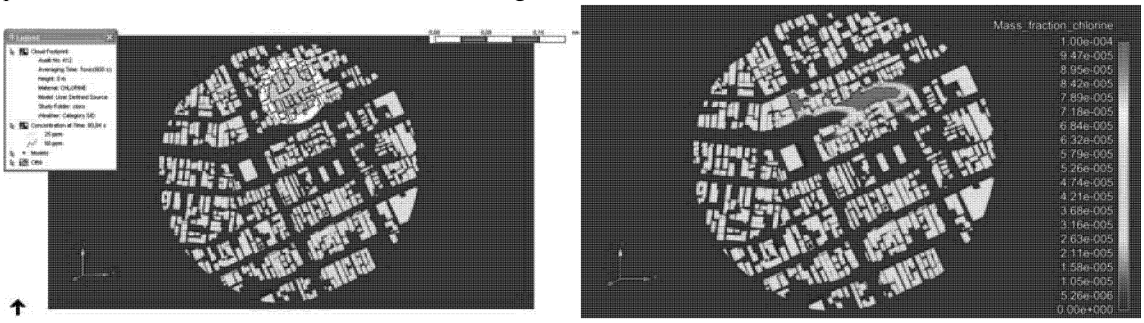


Figure 6. Sequence of images related to simulation with PHAST code.

6. 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 7.



(a) *(b)*

Figure 7 Comparison of the impact areas of the cloud after 80 seconds of simulation: (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 very 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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