# Dispersion of Accidental Release of $H_2S$ on a Gas production site followed in real-time by 3D modeling.

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## *Background and objectives*

The emergency actions following an accidental release of hazardous substance is strongly related to what is known of the accident and its evolution : the location of the source, the mass flow rate of the release, the velocity at which it is released and the duration of the release. These parameters, along with the atmospheric flows, will determine the spatial extent of the toxic cloud in time. While the major part of the planning is based on beforehand impact evaluation and experience, a real-time information, or rather a faster-than-real-time information, about the spread of the pollutant would therefore be extremely valuable information for the emergency crews both on site and in the possible inhabited areas around the site. To obtain such an information in time to take action upon it requires to be able to simulate the dispersion with fine precision and maximum speed. Precision can be brought by the computational fluid dynamics (CFD) simulations of the atmospheric flow to account for topography, turbulence, obstacles which standard Gaussian or integral models cannot provide. They tend to overestimate the concentrations and impact distances and are unable to simulate correctly concentrations at close range. However, the CFD simulations were known so far to be very time-consuming and hence could not comply with the requirements of a real-time operational simulation. A new methodology has therefore been developed and is detailed in this paper. A 3D CFD (Computational Fluid Dynamic) model (Fluidyn-Panepr) has been chosen, to simulate the 3D wind field pattern on the industrial site for a complete set of predefined boundary conditions based on the site windrose. These wind patterns have been stored and are automatically selected in case of an accidental release (triggered by detection of above-thresholds concerntrations at the sensors) by comparison with measurements carried out in the meteorological station located on the site. The location and intensity of the source term is determined using a probabilistic approach making use of both real time measurements and pre-calculated concentration responses from unitary emissions (puffs) on sensors. This approach was validated successfully using a limited number of sensors and sources on a complex site. The estimated source term is then used in forward dispersion mode to simulate the dispersion in (fast) Lagrangian puff mode. The industrial site of Lacq (France) has been chosen as a test platform and the key hazardous substance considered in this study is hydrogen sulphide ($H_2S$). The modeling platform will be validated through measurement campaigns with neutral species during the course of 2010.

## *A new methodology for faster-than-real-time simulation*

The following criteria for the numerical tool to be developed were defined :
- Precise simulation of atmospheric flow and toxic gas dispersion especially close to the source. Specifically, the following items should be accounted for :
  - Topography and obstacles (including porous obstacles such as pipe networks)
  - Variable wind conditions
- Simulation time should be faster than real time
- Inverse modelling to determine the source characteristics based on on-site measurements : location, transient mass flow rate, instant of emission.

A preliminary survey of existing tools showed that they are either unable to take into account the

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[1] TOTAL E&P
[2] FLUIDYN

detailed structure of the site (e.g. Integral/Gaussian dispersion models [1]) or could not provide a suitable source term determination algorithm. This suggested the need to develop a new approach. The general principle of this development is to couple in real time the sensor network of the industrial site with appropriate algorithm for source term determination and 3D dispersion modelling.

Fluidyn-PANEPR ([2][3][4]), a 3D CFD (Computational Fluid Dynamic) model has been chosen to simulate the 3D wind field pattern on the industrial site, taking into account the details of the installations. This model solves the Navier-Stokes equations for atmospheric flow in a RANS formalism. It includes mass, momentum and enthalpy conservation, state law and equations for advection-diffusion. A k-ε model in standard formulation is used for turbulence simulations and a micro meteorological model provides the initial atmospheric wind, turbulence and temperature profiles based on Monin Obukov similarity theory. This platform has been initially developed for consequence modelling of toxic/flammable atmospheric dispersion in complex industrial site[5][6] in a diagnostic risk assessment. In the frame of real-time modelling, the CFD model is used in Eulerian mode to calculate all 3D wind field patterns whereas a dedicated Lagrangian model is used more approprialtely for the calculation of dispersion of species. The precise description of 3D dispersion patterns is mandatory for the performance of the source retrieval module and highly valuable for the emergency and decision making on site.

The real time approach is made possible by the use of a complete database of pre-calculated 3D wind fields. In case of accidental release the 3D wind field will be automatically selected in order to match with the real time wind direction and speed measurements from the meteorological station located on the industrial site. The database will contain wind fields calculations for at least 60 different meteorological conditions covering the typical conditions of the site and when needed, the wind field will be calculated from interpolation between two conditions to match the real time conditions as close as possible.

Among the possible techniques for source term reconstruction, it was decided to use a probabilistic approach. Such technique is inspired by research activities in urban dispersion context of NRBC release [7][8][9]. Based on a field experiments in Urban 2003, the Bayesian inference method has proved efficient enough to recover location and intensity of a continuous release of neutral gas. Bayesian inference approach is also particularly suited when scarce and noisy data are likely. A specific module had to be developed in order to provide a most probable estimate of the location, intensity, and start-up time of the transient accidental release, based on the probability that a set of parameters values for a source term are responsible for a concentration field observed in real. The full range of parameters (location, intensity, release starting time and duration) is sampled in an optimised and converging random technique. Based on such sampling, a probability density function is produced for eachparameter. The advantage of this approach is its robustness with respect to noisy and scarce sensors and its fast delivery. This overall approach is fully automatic i.e. the activation of the simulation platform is triggered by the detection of above threshold concentrations at the sensors. The source term is then used in forward dispersion mode to simulate the dispersion resulting from the accidental release using Fluidyn-PANEPR model in Lagrangian puff mode. Since the production of 3D wind fields for both source term estimate and forward dispersion does not involve real time CFD calculations but ad hoc selection within a pre-calculated database, the computing time can be devoted to the retrieval algorithm (with sampling) and to the Lagrangian puff dispersion both fast enough and optimised. It is expected to be about 1/5 of the physical time of dispersion.

## *Implementation on the site of Lacq (France)*

In order to predict the most realistic evolution of a plume of gas in case of leak on a part of plant, a digital model of the Lacq site and its surroundings has been realised. The numerical representation of the site and its surrounding are shown in the following figures (figures 1 and 2). The overall area

includes the site of Lacq and its surroundings. (including inhabitated areas with villages). The size of the domain is 13.5 x 9.5 km. The size of the industrial site is about 1.8 x 1.3 Km. Two areas have been defined: the surrounding area where land use is described (i.e. woodland, urban area, rivers etc…) shown in Figure 1 ; and the industrial site itself where the details of buildings and installations have to be numerized (Figure 2). The second area is embedded in the first one (see Figure 1).
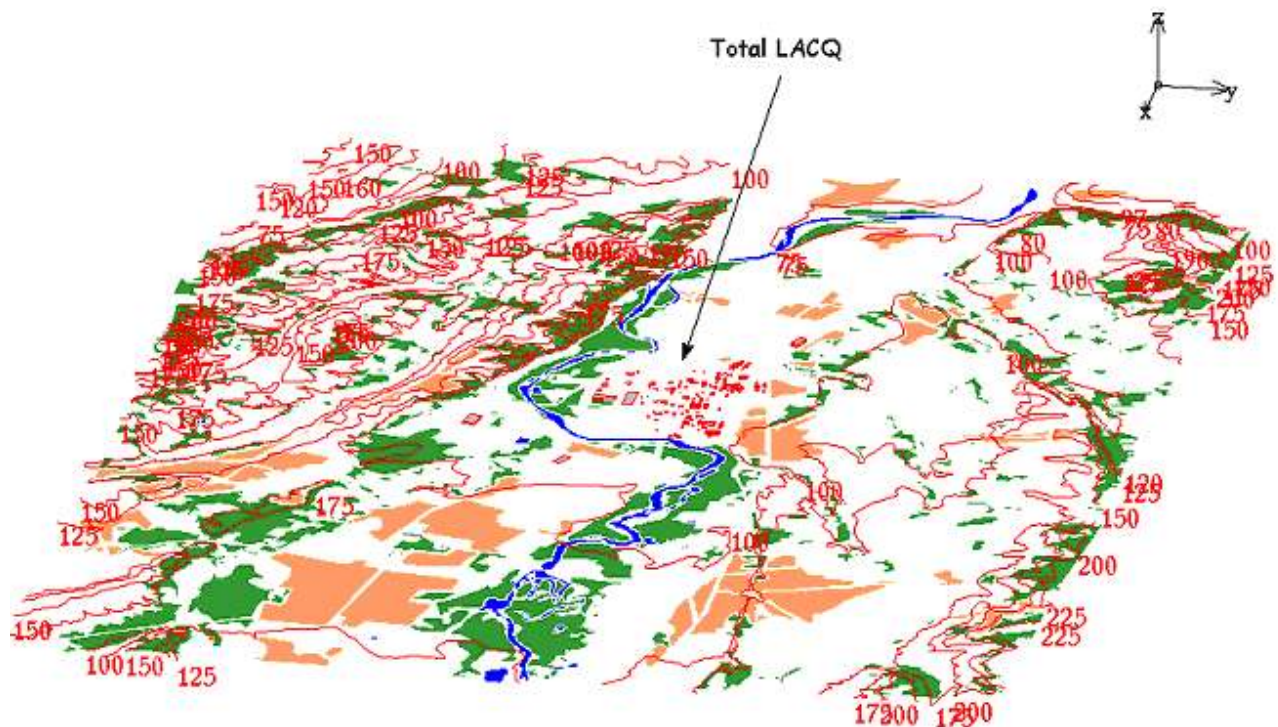


**Figure 1 : Numerical representation of the domain of interest : the industrial site of Lacq is located in the middle of the domain. In red, altitude contours, in blue, water bodies, in green, forests and in brown urban areas.**
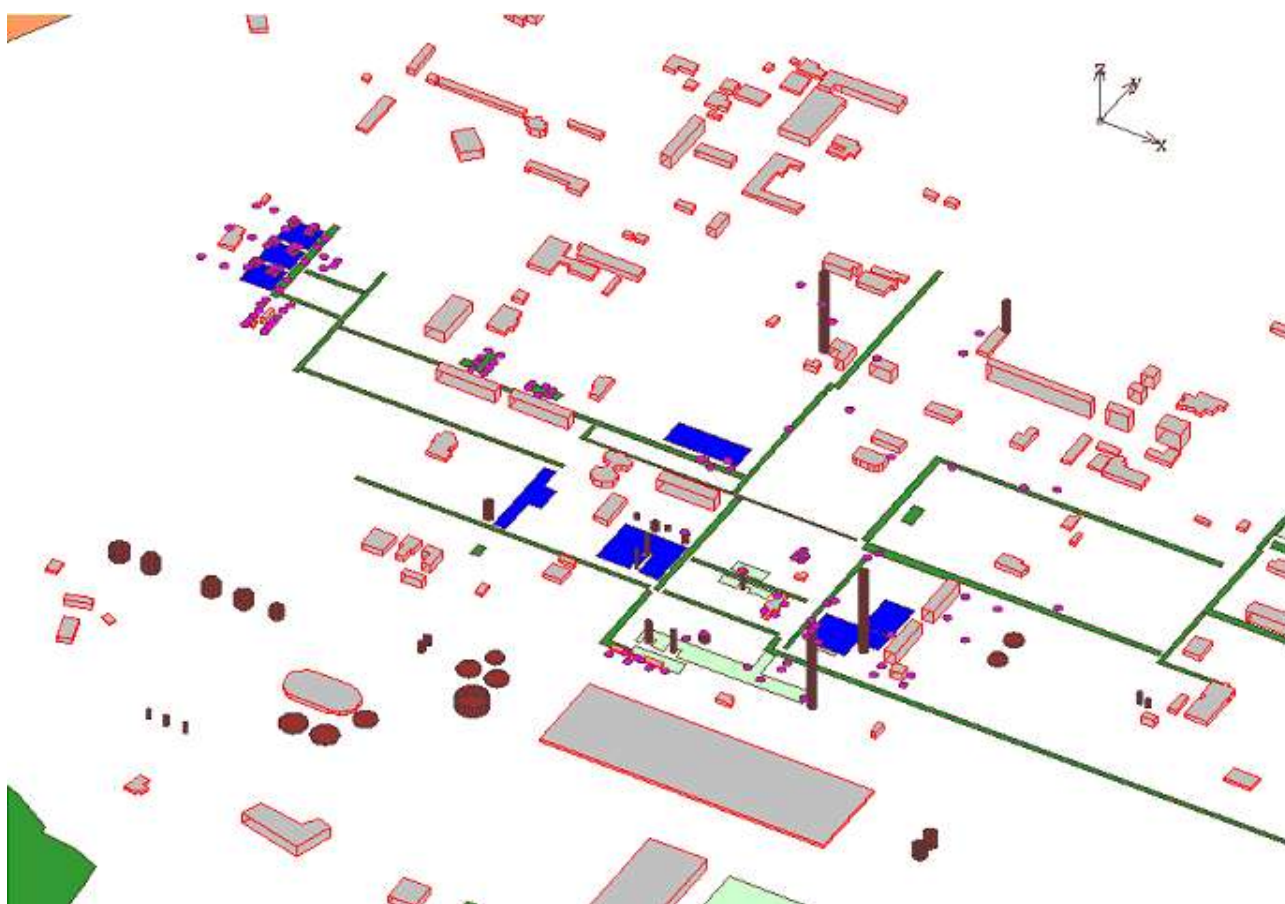
**Figure 2 : Zoom on the numerical representation of the site. Buildings are in gret, stacks and tanks are in brown, pipe networks are in dark green and process in Blue.**

In the first domain (large area in Figure 1) a detailed numerisation of building is not necessary at the exception of a few large building at the vicinity of the industrial site which required numerization. In this region far from the site, the influence of surface roughness on flow pattern is set through a rugosity coefficient coming from topographic maps, data from internal diagrams and additional data collected on the entire platform. All natural elements (altitudes, woods and forests, rivers ...) and all types of facilities that could interact with air flow were identified from GIS data (from French Geographical Institute IGN.). Actions inside and outside the factory were accomplished to collect dimensions and technical characteristics of buildings, technical facilities and outfalls that could modify the plume evolution (cooling towers, purge...). A final review on site of all installations defined and confirmed the size, morphology and features of the plants. For units heights, fast and reliable methods have been evaluated and two of them have been selected : the empirical method called "Thales" and the method by "Shadow" (measuring facilities shadows compared to a reference shadow taken at a date and reference time). An obstruction factor has been allocated to each installation to mimic their impact on the wind stream. A database was created for all these data collected on the Lacq platform.

Meteorological data and $H_2S$ concentration have to be available in real time configuration on the site. A meteorological station is installed on the site and has been tested to ensure the absence of interference with the installations. This station provides data on wind speed, direction and temperature and is linked to the information system of the process (PI) which is centralizing all the key information related to the process and sensors available on the site. On request to the system, the data are made available in real time in excel or csv file format. The site is also equipped with 178 $H_2S$ sensors. These sensors are either using electrochemical or semi-conductor detection

devices. The sensor data are collected by the PI system and can also be made available in real time in excel or csv file format. So far these detectors are used to trigger alarms and safety control systems at 5ppm (first level) and 10 ppm (Second level). They are used on the 0 to 20 ppm range and deliver analogue signal from 4 to 20 mA for the full range of concentration. All scenarios related to possible accidental release have been reviewed from the hazard study of the site. It enables an accurate determination of sources location and detailed composition of the emitted gas.

The mesh was optimized to ensure correct numerical resolution of transport and diffusion equations and also to match appropriately the detailed structure for the industrial site. For that purpose 3 modelling domains have been defined (Fig 3) and curvilinear mesh optimized. The smaller modelling domain with high resolution and unstructured mesh (mesh size between 1 and 10 m, see figure 4) is nested in an intermediate modelling domain with unstructured mesh (mesh size between 30 and 80 m) itself nested in the larger domain with structured mesh (mesh size between 60 and 150 m). Total number of cells is $1.6 \ 10^6$. The height of the domain is 300 m.
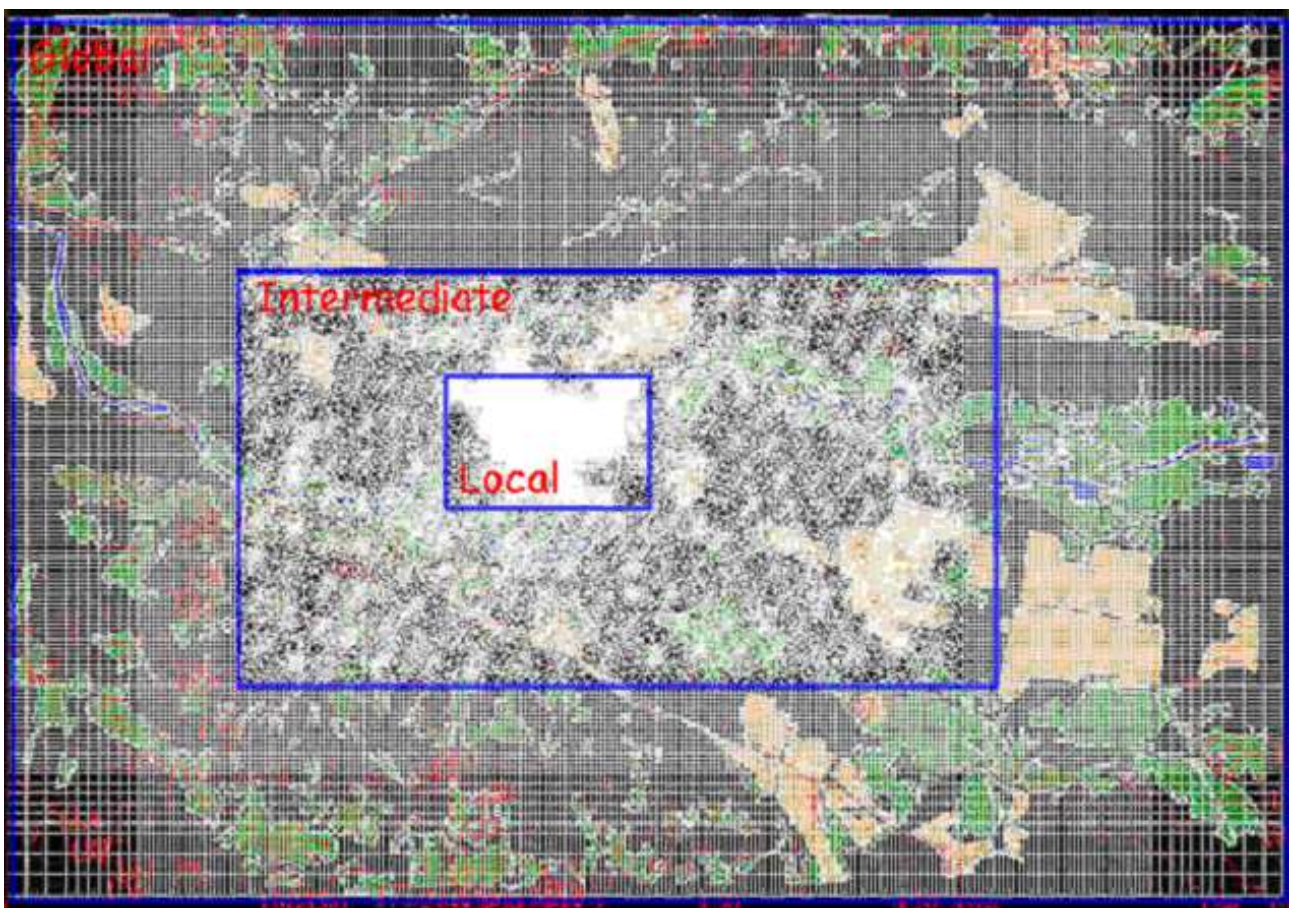


**Figure 3 : Top view of the 3 embedded mesh on the modeling domains.**
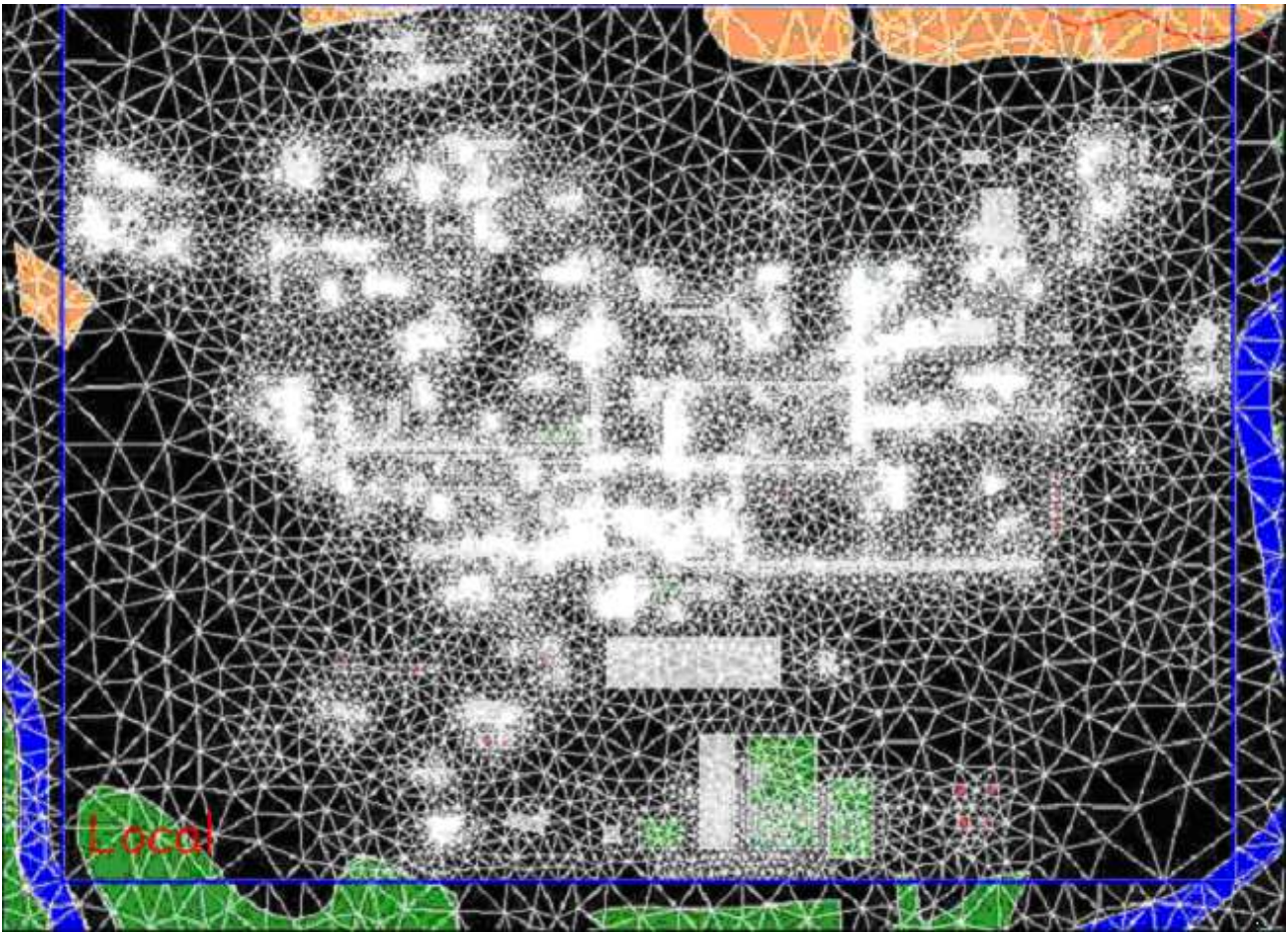
**Figure 4 : Top view of the finer mesh on the site domain.**

A survey of the wind directions and intensities carried out between 1992 and 1999 at the station of Lendresse (at 2 km from the site) was used to establish the frequencies of occurrence of wind conditions. This was used as the basis to establish 60 conditions in wind directions and intensity covering most of situations encountered on the site. So far 5 categories of wind intensities are considered between 0.5 and 8 m/s. All wind directions are considered by 20° direction steps. If wind conditions have to be simulated between two standard sets of conditions, interpolation is carried out to match the exact situation. These conditions have been applied as boundary conditions at the larger modelling domain to calculate each wind field pattern. Conditions for atmospheric stability are applied to simulate atmospheric temperature gradient expected in stable and neutral stability conditions. Further calculation will be conducted to cover all situations including atmospheric unstability conditions. An example of wind field calculation is illustrated in fig 5.(80°, 3 m/s).
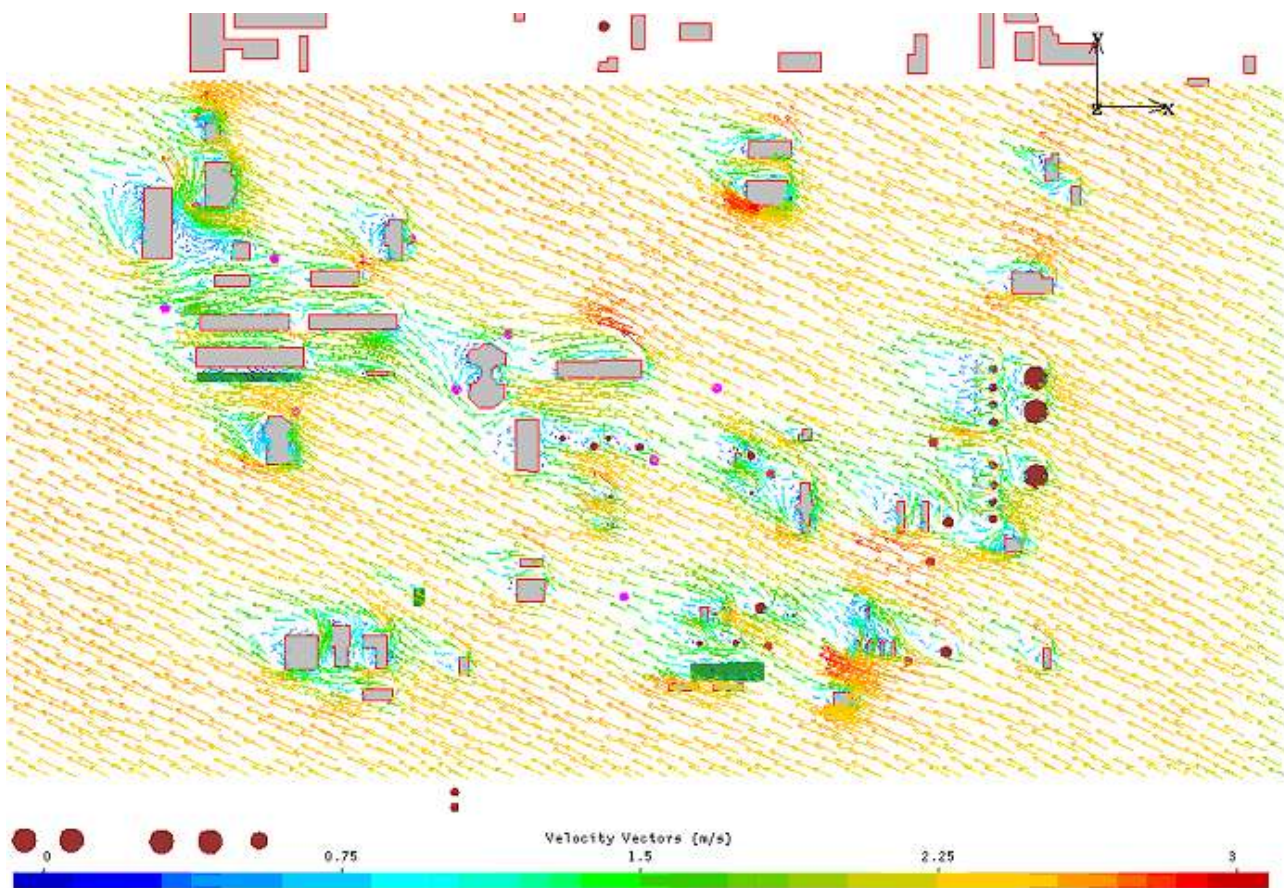
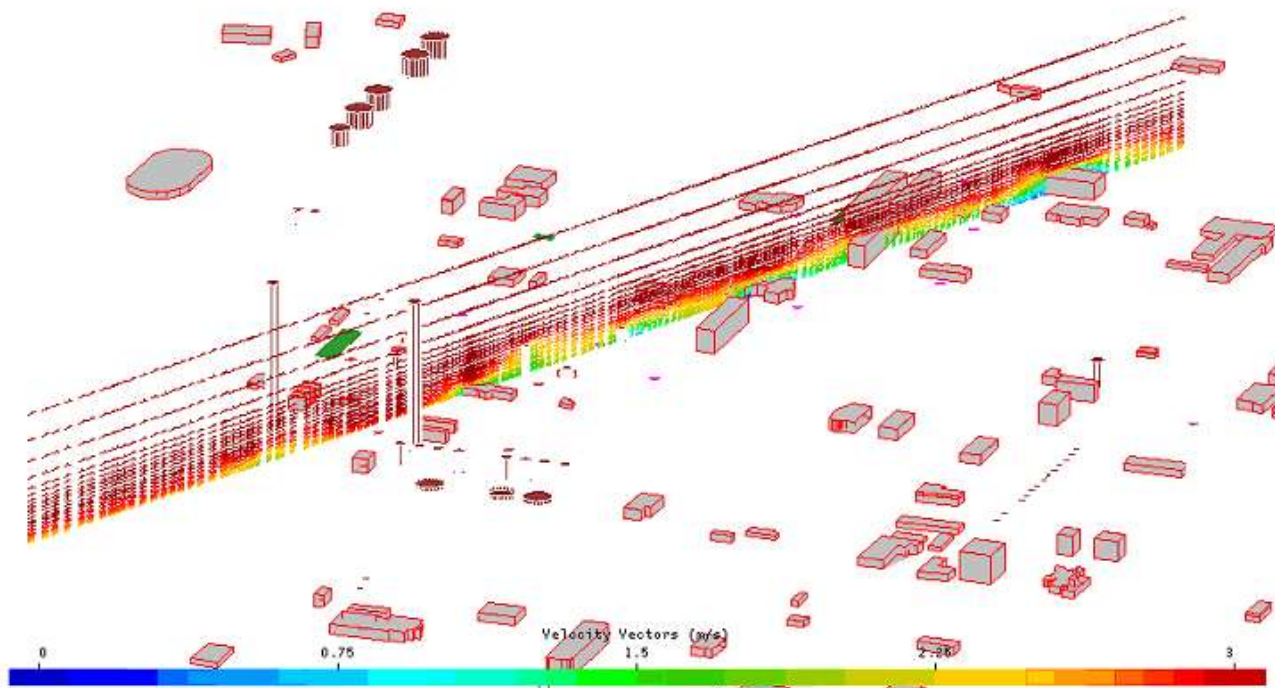**Figure 5 : Example of a windfield result (zoom on the site, top view of a plane at z=1.5m, velocity vectors)**



**Figure 6 : Example of a windfield result (zoom on the site, vertical section, velocity vectors)**

## *Source term determination examples*

Before full implementation, preliminary tests were conducted to validate the principle of the Bayesian algorithm. A numerical test with 5 potential sources and 10 $H_2S$ sensors were carried out using the detailed numerical representation of the site of Lacq on a part of the local domain. A domain of 1000 x 600 m was chosen within the local domain (Figure 7). In the case of this test the virtual accident correspond to a release with characteristics parameters:

- mass flow rate :       constant at 10 kg/s
- duration of leakage : 30s
- Source :                   n°4
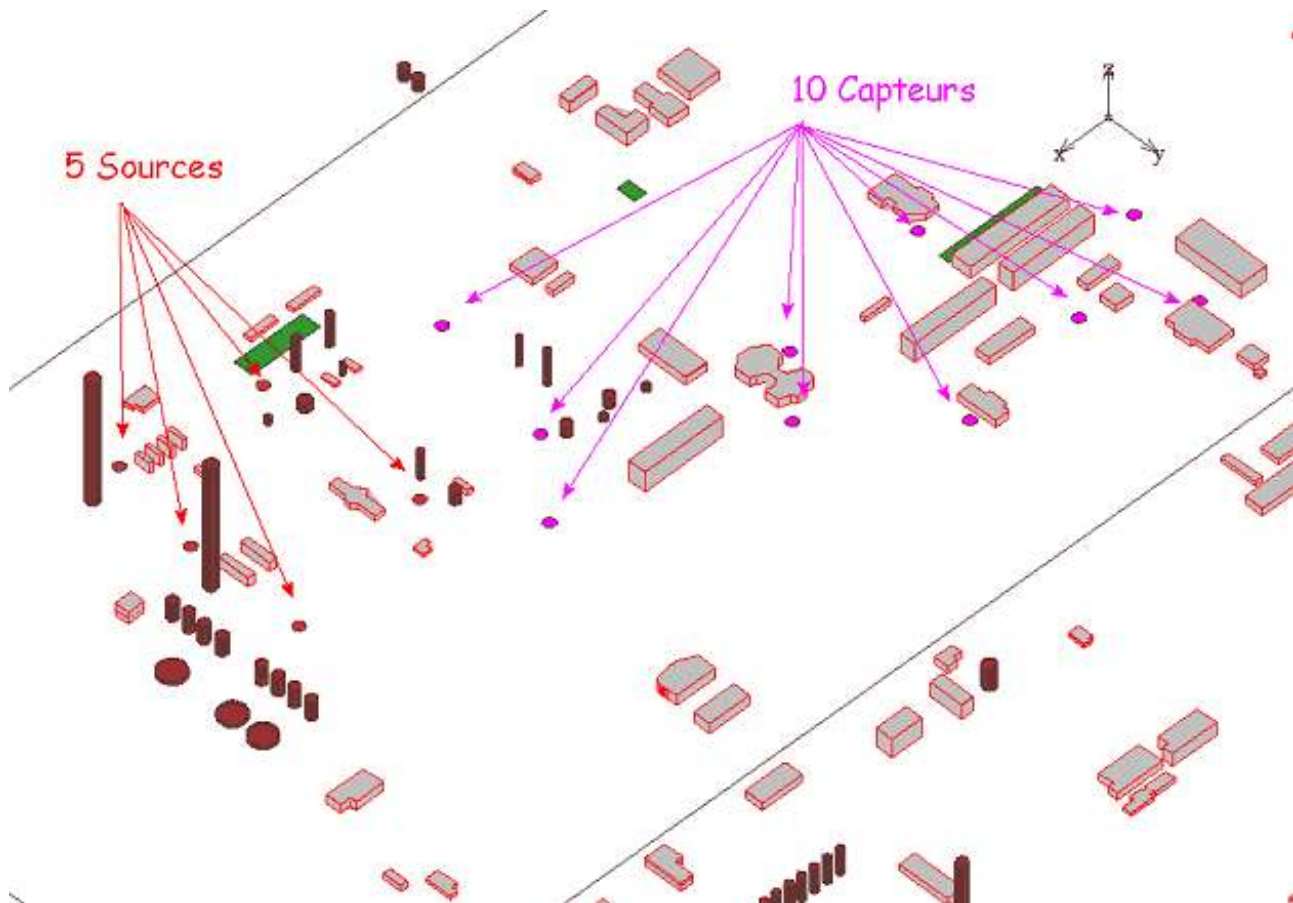- meteorological conditions with 3m/s speed @10mheight and 115°N directtion.



**Figure 7 : Local domain chosen for tests**

The direct forward synthetic responses on sensors are produced (Figures 8 and 9) with a numerical noise with a standard deviation of 10% as been introduced on the synthetic observed measurements to be as close as possible from real measurement variability (uncertainties and natural variability). The virtual detection (at 130sec after emission) is activated. The detection threshold is fixed at 5ppm with two measurements at the sensor for this case. The sampled values for the different parameters of the source are the location, the mass flow rate, the duration and starting time for the release. In this test case, the range for such parameters have been significantly narrowed in comparison with reality to facilitate the test. The ranges are 1 to 5 possible localizations, 0 to 60 kg/s for the mass flow rate,, 0 to 100 s for the duration and 0 to -300s for the starting time. The

sampling algorithm provided 40 000 propositions of parameters sets with related likelihood (based on the observed informations). A probability density function (PDF) is then reconstructed from such samples. The useful samples represent a small fraction of the global number of propositions; In this case they successfully identify the location 4 as the source. The identification of the location and probability density function for the mass flow are illustrated in Figures 10 and 11.
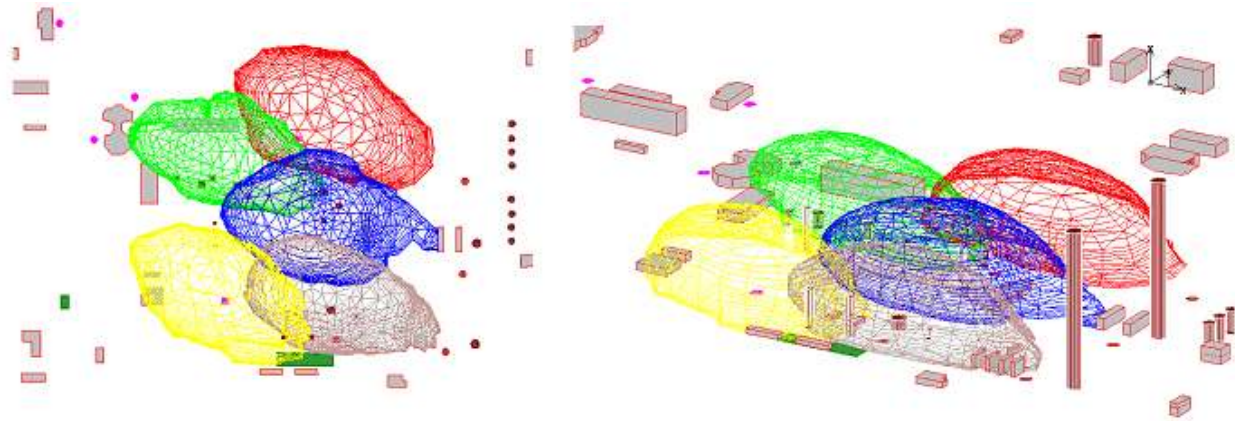


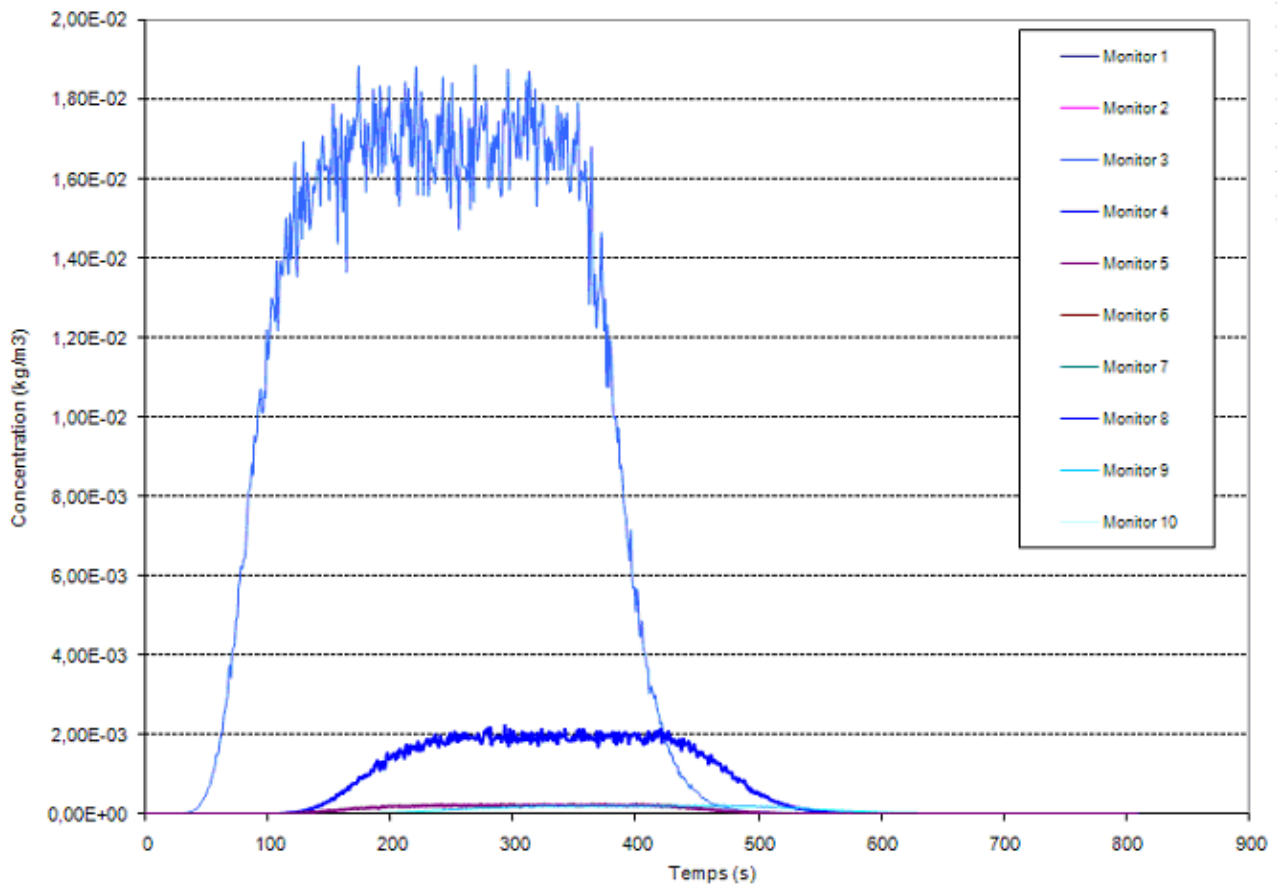**Figure 8 : Synthetic case of unitary emission coming from all sources to construct sensor response**



**Figure 9 : Synthetic response of sensors to an modelled emissions including numerical noise**
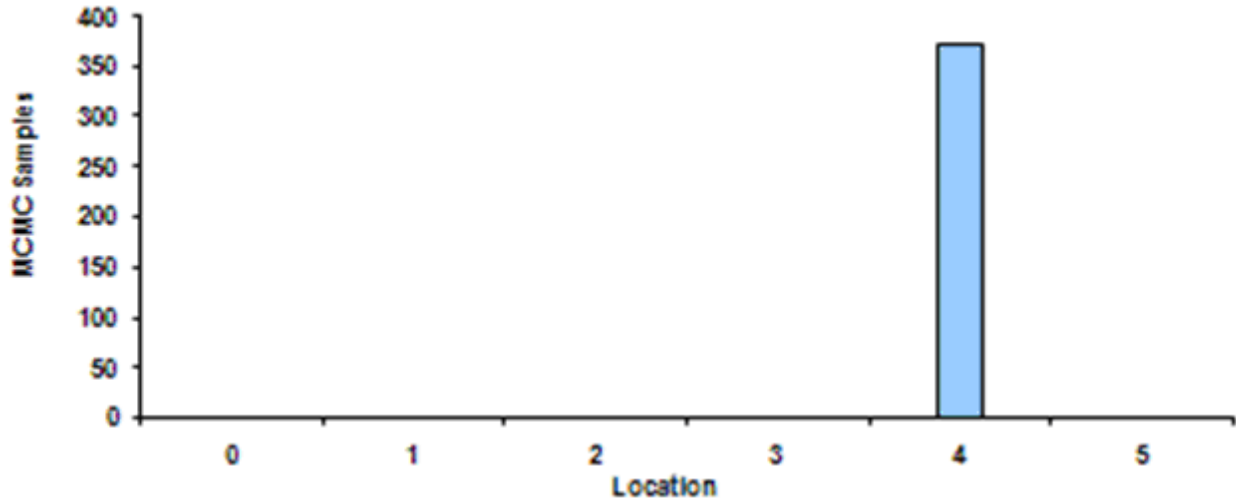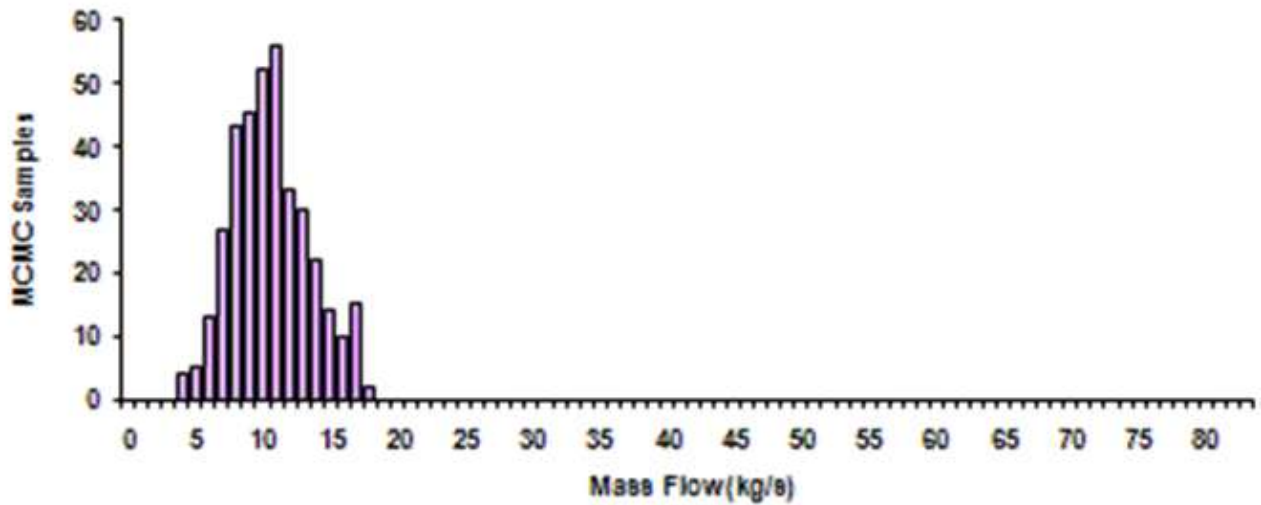
**Figure 10 : PDF for location**



**Figure 11 : PDF for mass flow rate**

Since in their present configuration the sensors range of concentrations is 0 to 20 ppm, no usefull information can be expected above these concentrations due to saturation. The inclusion of this measurement limitation in the retrieval process has been tested. In this case the sensors submitted to concentrations higher than 20 ppm are withdrawn from the sampling process although the historical data before saturation are kept. In this further test inclunding the sensor saturation, the sampling frequency of the signal at each sensor has been increased to every 5s.. The results obtained although less favorable are still satisfactory (see table: 1)

**Table I: Summary of results for bayesian inference of source parameters with and without sensor saturation effect.**

| | | Mass Flow (Kg/s) | Starting time (s) | Emission duration (s) |
|---|---|---|---|---|
| **Actual emission data** | | 10 | 130 | 30 |
| **Assuming no sensor saturation** | **Mean values from samples** | 11.9 | 120 | 48 |
| | **Average PDF Weighted values** | 8.9 | 123 | 45 |
| **With saturation of sensors** | **Mean values from samples** | 8.7 | 120 | 44 |
| | **Average PDF Weighted value** | 7.3 | 121 | 30 |

## *Conclusions*

Some of the key elements of the modeling platform dedicated to the real time simulation of accidental release on industrial site have been tested successfully. The infrastructure on the site of Lacq enables real time acquisition of meteorological and $H_2S$ data. The density of sensor is at an acceptable level for detection and source reconstruction. Wind field simulation was carried out satisfactorily at high resolution. Three modeling domains have been defined and nested in each other with the proper grid structure to optimize the numerical resolution of advection and turbulence terms for both the industrial site and the surrounding domain (up to 10km) . Bayesian inference with a random sampling approach was successfully used to determine the source term in the complex situation of building and structure of the industrial site. Some more work is needed to extend the database of pre-calculated wind field to take into account the detailed micrometeorology of the site of Lacq. Also the Bayesian inference algorithm will be expanded to the full local domain. Finally a validation campaign using a neutral species will be conducted. The first phase of that campaign will take place in March 2010. The second phase is likely to be carried out in summer in 2010 or 2011.

## *Acknowledgement*

## *References:*

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