Real Time Simulation of the Dispersion of Accidental Emission Release of Hazardous Substance on Industrial Site Using 3D Modelling.

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Abstract

The knowledge in real time of the concentration fields resulting from the accidental release of hazardous substance would be extremely valuable information as support for emergency actions and impact evaluation on the industrial site itself and its vicinity. For that purpose, a modelling platform is being developed and applied to simulate in real time the atmospheric dispersion of hazardous substance at the scale of the industrial site and also on its surroundings. The industrial site of Lacq (France) has been chosen as a pilot and the key hazardous substance considered in this study is hydrogen sulphide (H_2S). A 3D CFD (Computational Fluid Dynamic) model (Fluidyn-Panepr) has been chosen, to simulate the 3D wind field pattern on the industrial site, taking into account the details of the installations. This approach enables a simulation as close as possible of the turbulence and flow around the buildings which could not be done with a standard Gaussian approach. For that purpose a detailed numerical model of Lacq installation was built based on a thorough review of the existing installations and evaluation of their size and porosity. Wind fields were calculated for a set of predefined boundary conditions based on the climatology of the site. Investigations were carried out to ensure that site Information Systems could deliver in real time the information available from the H_2S sensors and on site meteorological station. The real time approach is made possible by the use of complete wind field pre-calculated database automatically selected in case of accidental release by comparison with real time wind direction and speed measurements from the meteorological station located on the industrial site. The location and intensity of the source term is determined using a probabilistic approach (Bayesian inference) 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 but with the complex structure and flow patterns expected on the site. The activation of the simulation platform is triggered by the detection of above threshold concentrations at the sensors. The estimated source term is then used in forward dispersion mode to simulate the dispersion in (fast) Lagrangian puff mode. The modelling platform will be validated through measurement campaigns with neutral species in 2010.

Introduction

On industrial installations devoted to oil and gas extraction, processing, refining or petrochemical production, accidental releases of toxic compounds represent a significant part of the risks related to these activities. When such an accident occurs, the knowledge in real time of the concentration fields resulting from the release of the hazardous substance would be extremely valuable information as support for emergency actions and impact evaluation on the industrial site itself and its vicinity. For that purpose, a modelling platform is being developed and applied to simulate in real time the atmospheric dispersion of hazardous substance at the scale of the industrial site and also on its surroundings i.e. from 5 to 10 km in any direction. The industrial site of Lacq (France) specialized in gas production has been chosen as a pilot for this project because of a favourable infrastructure in terms of network of sensors and meteorological stations availability. The key hazardous substance considered in this study is hydrogen sulphide (H_2S). Significant technical difficulties have to be solved to develop successfully this project: the calculation of the dispersion must take into account the real structure of the installation to correctly simulate concentration fields on the industrial site, the location and intensity estimation of the accidental release have to be done automatically by the modelling platform and calculation must be done in a few minutes to enable real time use of data. A preliminary survey of existing tools showed that they are either unable to take into account the detailed structure of the site (e.g. Integral/Gaussian dispersion models, [1]) or do not provide a suitable source term determination algorithm. This

suggested the need to develop new approaches. The general principle of this development as illustrated in fig.1 is to couple in real time the sensor network of the industrial site with appropriate algorithm for source term determination and 3D dispersion modelling. The project is divided in two phases: a first phase devoted to the development of the modelling platform and its implementation on the industrial site and a second phase devoted to in situ validation of the CFD model with an atmospheric tracer (SF_6) which is planned for year 2010. In this paper it is intended to present the results and conclusions obtained during phase 1 of this work.
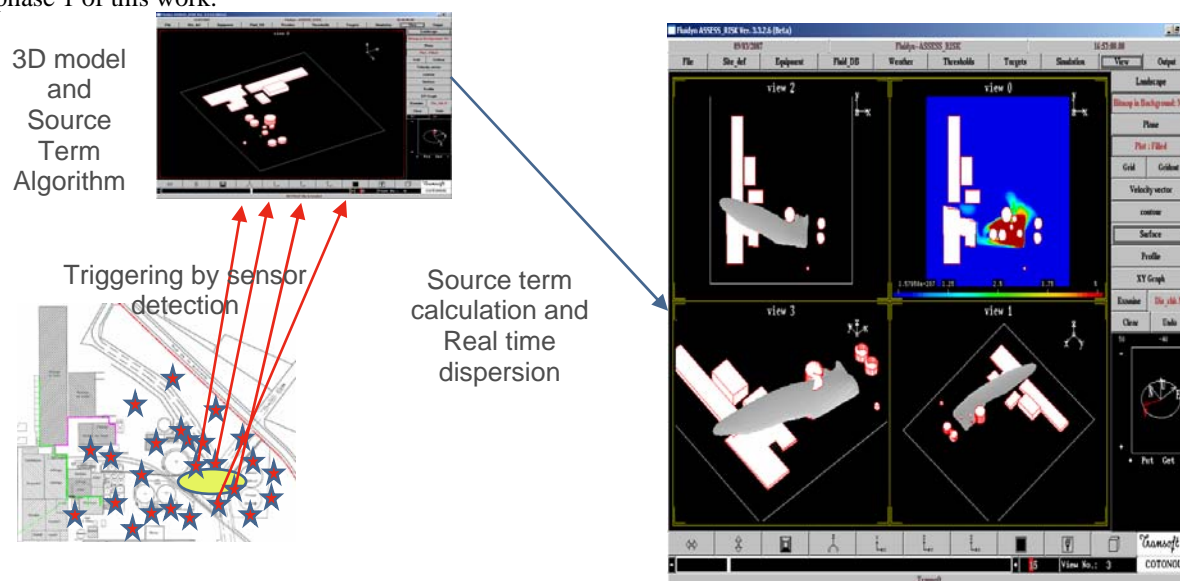

3D model
and
Source
Term
Algorithm

Triggering by sensor detection

Source term calculation and Real time dispersion

Figl: General principle

Statement of theory and definitions

A 3D CFD (Computational Fluid Dynamic) model (Fluidyn-Panepr, see [2][3][4]) 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 appropriately for the calculation of dispersion of species. In this project incompressibility assumption is made for flow pattern calculations and a buoyancy model is used to simulate heavy gas behaviour. This approach enables a simulation as close as possible of the turbulence and flow around the buildings which could not be done with a standard Integral or Gaussian approach which tends to overestimate the concentrations and impact distances and is unable to simulate correctly concentrations at close range. 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 drawback of CFD calculation is that it requires large CPU time. Therefore, 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 experiment in Urban 2003, the Bayesian inference has proved to be efficient enough to recover location and intensity of a continuous release of neutral gas. In the project presented below a specific module had to be developed to provide a most probable estimate of the location, intensity, and start-up time and duration of the transient accidental release. Bayesian inference approach is particularly suited for such applications in industrial context where scarce and noisy data are likely to be available. The probability that a set of parameters values for a source term be responsible for a concentration field observed in real time is built from differences between observed concentration at each sensor and pre-calculated concentration data for each possible source. A database for the sensors responses (in time) to unitary emission (puffs) from the plausible source locations and 3D flow patterns is developed for the specific source recognition algorithm. The responses matrix thus archived are used in real time within the inference algorithm. 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 each parameter thus enabling to identify the most probable properties of the source term. The advantage of this approach is its robustness with respect to noisy and scarce sensors and its fast delivery. As far as the sensors network is embedded in the industrial units and buildings, a reliable estimate of the likeliest scenario from the Bayesian approach needs precise simulations of complex wind flows and dispersion patterns as provided by CFD calculations. 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 calculated by this approach 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.

Description and application of Equipment and Processes

Numerical representation of the site

In order to predict the most realistic evolution of a plume of gas in case of leak on a part of the plant, a digital model of the Lacq site and its surroundings has been realized. The overall area includes the site of Lacq and its surroundings. (See FigIIa) (Including inhabited areas with villages). The size of the domain is about 13.5 x 9.5 Km and the size of the industrial site is about 1.8x1.3 km. Two areas have been defined: the industrial site itself where the details of buildings and installations have to be digitalized and a second area where a detailed digitalization of buildings is not necessary at the exception of a few large buildings at the vicinity of the industrial site. In the second area the influence of surface roughness on flow pattern will be treated through a roughness coefficient taking into account land use i.e. urban area, woodland etc... All natural elements (levels, woodland, rivers ...) and all types of facilities that could interact with air displacement were derived from GIS data (from French Geographical Institute IGN.). Actions inside and outside the factory were made to collect dimensions and technical characteristics of buildings, technical facilities and gaseous emissions able to modify the plume evolution (cooling towers, purge...). Regarding the facilities sizing, internal data sheets and records have been used. In case of lack of data for heights of units, fast and reliable methods have been evaluated and two of them have been selected: either using Thales principle or the shadow of installations (measuring facilities shadows compared to a reference shadow taken at a date and reference time). In each case building with well known heights were used as validation check. An obstruction factor has been allocated to each installation to best reflect their impact on the wind stream. The term of "porosity" was then used to characterize the ability of certain structure to allow part of the flow to go through. The work made in the periphery of the plant (notification of facilities, exhaust) has also been a significant part of the data collection work. A final technical visit was made to confirm the size, morphology and features of the plants. The numerical representation of the site and its surrounding are shown in Fig (IIa and IIb).
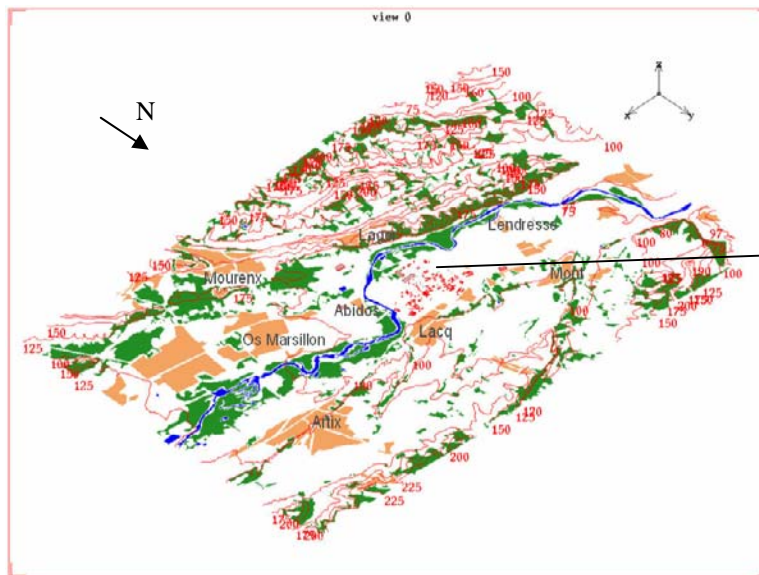

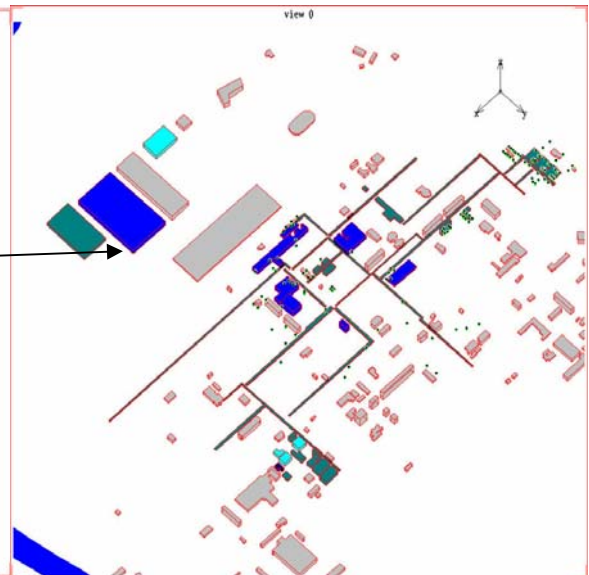**Fig II a: Numerical representation of the global domain**   **Fig II b: Numerical representation of the local domain**

Technical configuration for real time simulation

Meteorological data and concentration from the network of H_2S sensors have to be available in real time configuration on the site. A meteorological station is installed south side of the "Utilities power plant" 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.

Data and results

Wind field calculation.

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 IIIa) and curvilinear mesh optimized. The smaller modelling domain with high resolution and unstructured mesh (mesh size between 1 and 10 m, Fig IIIb) 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) (see Fig:IIIa) Total number of cells is $1.6 \ 10^6$. The height of the domain is 300 m.
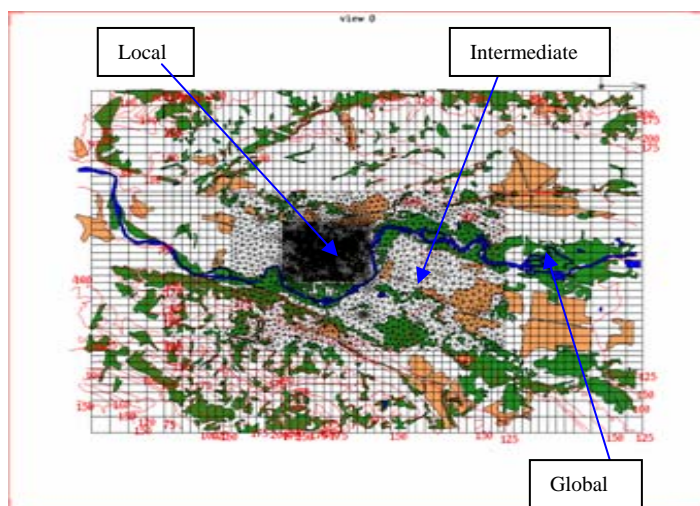

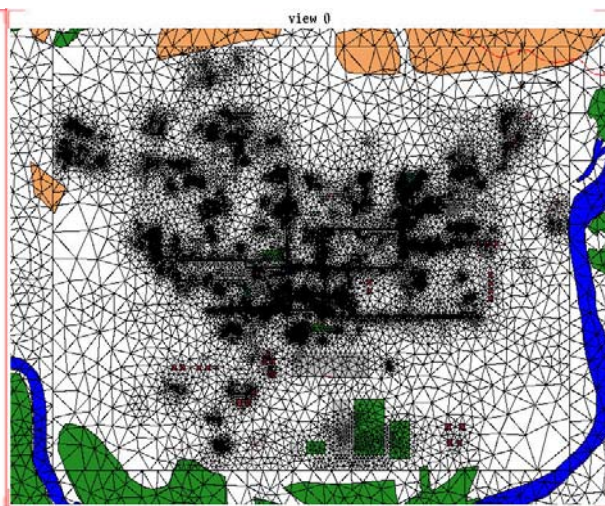**Fig III a: Mesh and modelling domains definition**

Fig III b: details of the Mesh for the local domain.

A survey of the wind directions and intensities carried out between 1992 and 1999 at the station of Lendresse (North-West location at about 2.5 km of the site) was used to establish the frequencies of occurrence of wind characteristics. The site is located in the Gave de Pau river valley. Altitude is about 90 m above see level and the valley is sided by higher altitude locations like Lagor at about 200m above see level. Dominant winds are from south west and west directions. These data were 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 to standard sets of conditions, interpolations will be 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

Fig IV: Example of wind field calculation at 0.25 m height.

applied to simulate atmospheric temperature gradient expected in stable and neutral stability conditions. Further calculations will be conducted to cover all situations including atmospheric instability conditions. An example of wind field calculation is
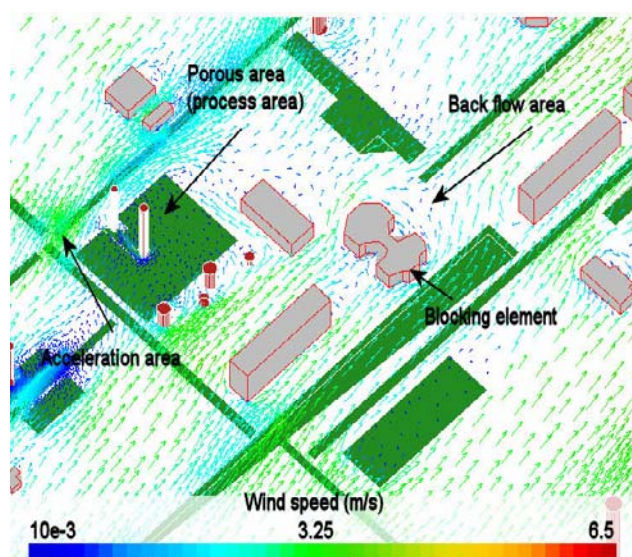
illustrated in fig: IV (80°, 4.5m/s,0.25 m height).

Source term determination

Before full implementation, preliminary tests were conducted to validate the principle of the Bayesian algorithm. Initially a very simple configuration test with 5 potential sources and 3 sensors and no numerical representation of the installation was conducted successfully. A second series of tests was carried out using the detailed numerical representation of the site of Lacq on a limited area of the industrial site. A domain of 1000 x 600 m was defined within the local domain with 10 H_2S sensors and 5 potential sources. So far this configuration is arbitrarily determined with the objectif to test the inference algorithm in a complex situation basically identical to the fully detailed configuration. (See fig Va).
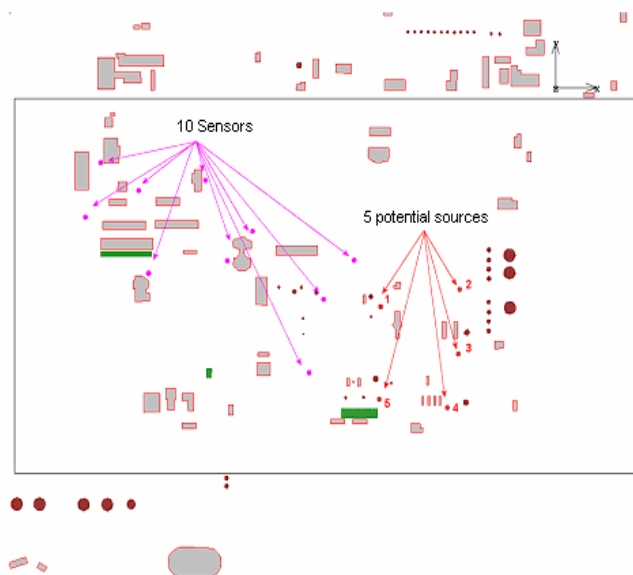

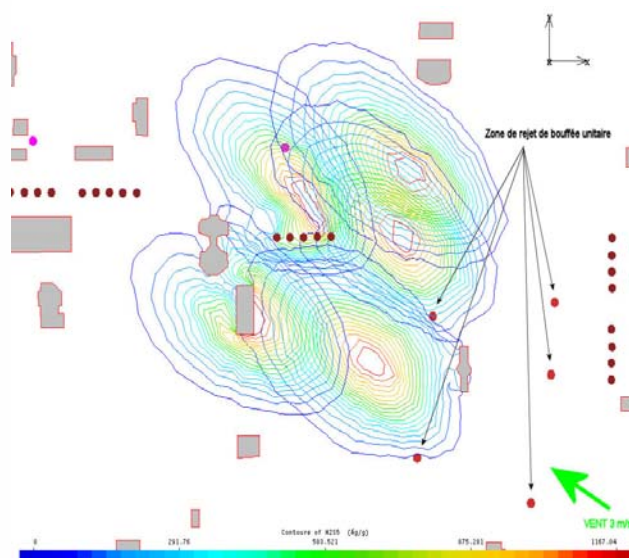**Fig: Va: Limited modelling domain for algorithm test.**

Fig: Vb: Example of unitary puff dispersion for the inversion database

A database with concentration fields resulting from unitary puffs (see Fig.Vb) was constructed for the 60 meteorological conditions as discussed in above section. In the case of this test the virtual accident corresponds to a release with characteristics parameters: mass flow rate- 10 kg/s, duration: 30s from source N°4 and meteorological conditions of 3m/s speed at 10 m height and 115°N direction. The direct forward synthetic responses on sensors are produced (Fig. VI) and the virtual detection (at 130sec after emission) is activated. The detection threshold is fixed at 5ppm with two measures at the sensor for this case (See vertical bars on Fig. VI). 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: 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 40000 propositions of parameters sets with related likelihood (based on the observed information as shown in Fig VI). A probability

Fig VI: concentration at sensor location.

density function (PDF) is then reconstructed from such samples. For this case, a numerical noise with a standard deviation of 10% has been introduced on the synthetic observed measurements to be as close as possible from the real measurement variability (uncertainties and natural variability). 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
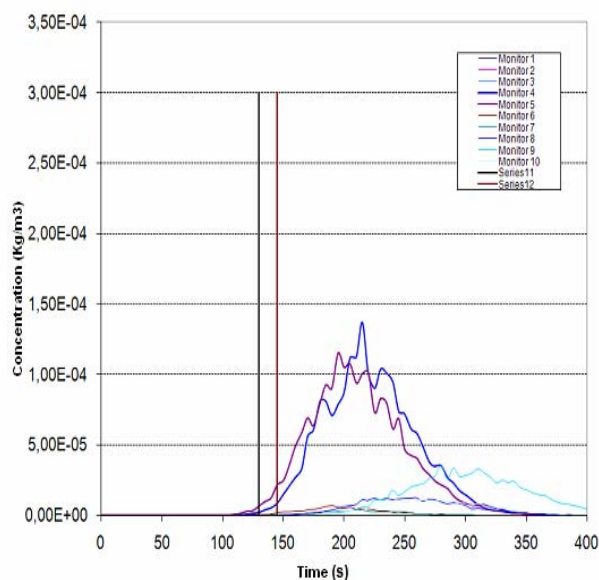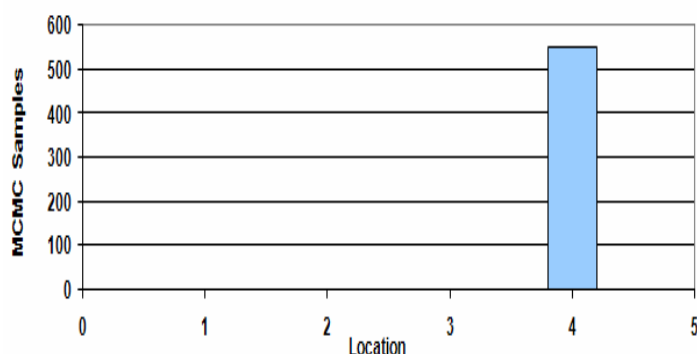
Fig VII: Localization of the source through sampling. **Fig VIII: PDF for mass flow rate.**

of the location and probability density function for the mass flow are illustrated in Fig VII and Fig VIII. It shows that the average (probability weighted) value for mass flow rate is 8.9 Kg/s with a target of 10 kg/s. Similar approach gives estimations for starting time and length of the accidental release. The results obtained show a very good agreement (See Table I). In their present configuration, the sensors range of concentrations is 0 to 20 ppm and no useful information can be expected above 20 ppm because of 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 including 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: I)
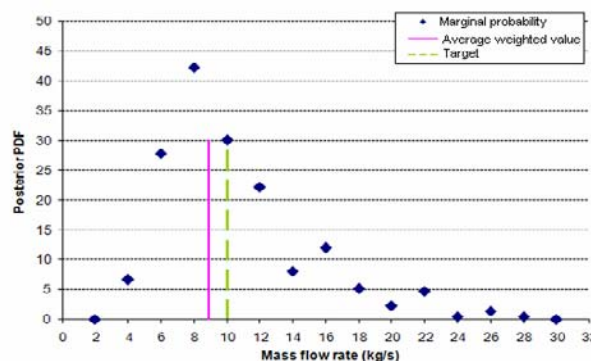
		Mass Flow (Kg/s)	Starting time (s)	Emission duration (s)
Assuming no sensors saturation	Mean values from samples	11.9	120	48
	Average PDF Weighted values	8.9	123	45
With saturation of sensors	Mean values from samples	8.7	120	44
	Average PDF Weighted value	7.3	121	30
	target	10	130	30

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

Conclusions

Some of the key elements of the modelling 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 sensors is at an acceptable level for detection and source reconstruction. Wind field simulation was carried out satisfactorily at high resolution. Three modelling 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. Bayesian inference with a random sampling approach was successfully used to determine the source term in synthetic cases using 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:

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