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VALIDATION CAMPAIGN OF A CFD TOOL ON A PETROCHEMICAL SITE WITH WIND FLUCTUATIONS INTEGRATION

Jean-Marie Libre[1], Stéphanie Guérin[1], Brahima Konaté[1*], Aldo Castellari[1*], Cédrick Mames[1*], Malo Le Guellec[2] Thibault Mailliard[2], Amita Tripathi[2],Claude Souprayen[2], Olivier Connan[3], C. Leroy[3], P. Laguionie[3], P. Defenouillère[3], B. Letellier[3], D. Hébert[3], Denis Maro[3]*

[1]TOTAL E&P, Paris- La Défense,[1*]TOTAL E&P Lacq, France
[2]FLUIDYN France, Saint-Denis, France
[3]IRSN, Cherbourg-Octeville, France

Abstract:Two measurement campaigns (12th-24th of March 2010 and 10th-22th of February 2011) have been carried out on the TOTAL site in Lacq (FRANCE) for different kind of SF_6 releases. The statistical analysis of the spatial gas concentration distribution and of the meteorological data (wind speed, wind direction, temperature, TKE, Monin-Obukhov length) collected on the TOTAL Lacq site at one point (mast) and on two other meteo stations in the surrounding villages has shown classical unsettled meteorological conditions during the trace gas emission.
The microscale short time natural wind fluctuations, as observed, can be qualified by two criteria:

1- the averaged behavior (constant velocity and direction) of the flow considered as steady. The averaging time for such characteristics is around 10 minutes.
2- the short time variations (seconds to several minutes) around the mean value which are therefore tricky to model in details.

The main objective of the campaigns was to understand the cloud motion in complex industrial configuration. This campaign takes a major place in a software development for real time accidental impact on industrial site. The numerical basis of this tool is the CFD software Fluidyn-PANACHE which models the gas and particles atmospheric dispersion taking into account the topography and 3D obstacles. A finite volume based approach is applied in which the governing differential equations for mass, momentum and heat transfer are solved in 3D space and time.
The sampling duration of the concentration records at the 15 sensors (9 minutes) requires a special modeling of the meteorological conditions by the CFD tool. A high frequency sampling of the meteorological data had to define the boundary conditions of the CFD simulations in association with an unsteady calculation of the 3D gas dispersion by an eulerian solver. Comparison between observed and simulated concentrations has been performed for several sequences of observations periods (around 10 different releases distributed in the diurnal most active times). It shows that the proposed CFD approach captures/reproduces enough natural variability to achieve good results for trends and mean values and little deviation figures between model and measurements.

Key words: *dispersion modelling, CFD, experimental campaign, comparison, petrochemical site*

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 potential hazards. In case of such an unfortunate event, the extent of human and material losses depends a lot on the detection speed and subsequent intervention. In this context, a numerical tool has been developed in collaboration with TOTAL in the framework of CITEPH (Concertation pour l'Innovation Technologique dans l'Exploration et la Production des Hydrocarbures) to predict in real time the drift of a toxic cloud accidentally released on an industrial site and the expected toxic concentrations on a region covering the site and its surroundings. In order to be used in emergency situation response, the simulation should run faster than the evolution of accident, while in operation (Libre et al, 2009), (Libre et al, 2010).

The framework of the intended use of the software requires simulations of atmospheric flows and dispersion of toxic species accurate enough to deal with the complexity of the industrial site as well as robust and fast.In earlier communications, it was determined that the 3D CFD deterministic models are the best-fitted models for accuracy of wind flows. Indeed, the wind and turbulence variations over the terrain and dispersion are computed based on the full fluid dynamics equations discretized on a finite number of spatial points, the mesh. The finer the mesh and the higher the numerical scheme order, the closer the solution is to real atmospheric flow but the higher is also the CPU time. The CFD tool used for this study is the standard version of Fluidyn-PANEPR®. (Fluidyn-PANACHE 2008), (Tripathi et al, 1994), (Hill et al, 2007), (Mazzoldi et al 2008).

To understand the cloud motion in the complex industrial configuration and to compare with results obtained numerically, two experimental campaigns (March 2010 and February 2011) have been carried out on the gas extraction platform of TOTAL located in Lacq for several SF_6 releases. A comparison of simulations with observations has been performed for several sequences of observations periods (around 10 different releases distributed in the diurnal most active times). Some of the results are presented here.

In the first section, a description of the experimental campaign is given. The second section provides the details regarding the numerical model and finally, the third section compares some of the results obtained experimentally with the numerical values for concentration.

EXPERIMENTAL CAMPAIGN

The gas extraction platform of Lacq is located at about 25 km from Pau, South-West of France, in a valley with some significant relief around it. Two experimental campaigns of SF_6 release and measurements have been performed by IRSN in February 2010 and March 2011 (Connan et al, 2010). The significant results from the first campaign are presented and discussed here.

During this experiment, weather data were collected by three YOUNG ultrasound anemometers (for temperature, wind speed, wind direction and turbulent fluctuations) and one AHLBORN weather station (for pressure, temperature, humidity, wind velocity and direction, rainfall and global radiation) located at 10m high in 3 different locations: on site, at the bottom of the valley and on the mountain above the site. Weather data (temperature, wind velocity, humidity, wind direction) recorded by averaging on an interval of 10 minutes with a frequency of 10 records per minute. From the recorded data, Monin-Obukhov length, roughness length, friction velocity and sensible heat flux were derived.

For each experiment, a pressurized bottle of SF_6 was equipped with a manometer, a gas flowmeter and was positioned on a scale to derive the total mass released into atmosphere. The SF6 was released through a flexible pipe to the specified location. Emission duration varied from 10 to 30 minutes with a constant mass flow rate (1.4 to 5.9 $g.s^{-1}$ depending on the experiment). The air sampling was carried out with two automatic gas sampling systems designed by IRSN named DIAPEG or EA.DIAPEG systems fill during 9 minutes from 2 to 5 sampling bags. The EA systems are easierto set up but do not allow for sampling over a long period of time and contain only two bags. Bags are made of Tedlar® (Polyvinyl Fluoride) considered to be inert and with no significant loss of gas during the experiment. For each experiment 15 DIAPEG and 12 EA can be used. Sampling points are distributed on site within the industrial structures and in some cases outside the industrial site. Distances for sampling range between 50 and 2500 m. SF6 analysis are carried out by Gaseous Phase Chromatography with Electron Capture detection (AUTOTRAC 101 Tracer Gas Monitor). The detection limit was estimated to be 25 ppt with a 3% precision for the scale (0-10 ppb). Only the values above 50ppt were considered. The time needed for one measurement is 2 minutes.

During the February 2010 campaign, the weather was very dry with low wind speeds. The wind directions have varied a lot during the entire campaign. The table 1 shows data for 2 tests that have been used for comparison with numerical results.

Table 3. Experimental set-up for three tests on site

Test case	**SF_6mass flow rate (g/sec)**	**Durationof release (min)**	**Emission height (m)**	**Number of samplings**
1	1.7	10	2	3 with 13 DIAPEG, 2 with 15 EA
2	1.8	30	1	3 with 13 DIAPEG

NUMERICAL MODEL

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 model solves the Navier-Stokes equations including mass, momentum and enthalpy conservation, state law and equations for advection-diffusion in a finite-volume-based approach on a non-uniform mesh generator that accounts for the presence of obstacles or topographical features (i.e. with generation of a finer mesh in critical areas). A k-ε model is used for turbulence simulationsand a micro meteorological model simulates the atmospheric temperature profile based on Monin Obukov similarity theory. This model is used in Eulerian mode for this comparison exercise. Boundary conditions (wind direction, speed, temperature and turbulent parameters) are based on measured data from the 10m height mast located on site at a place where no significant structure influence is expected. The wind speed and air temperature profiles are represented by logarithmic functions. The micrometeorological parameters are evaluated for different atmospheric stability classes.The ground roughness is set-up using a condition within which the wall shear stress and heat transfer in the boundary layer are computed from the standard logarithmic law of the wall, and introduced into momentum and energy equations.

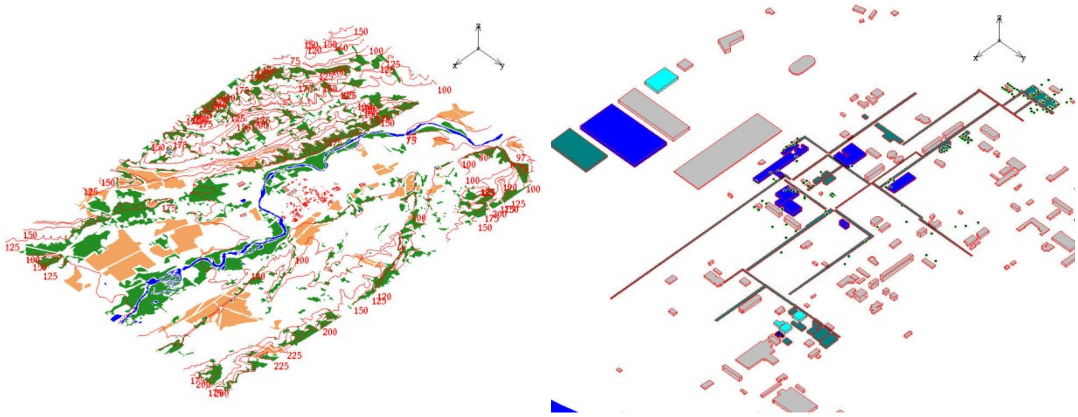

Figure 5. Numerical model of entire domain (left side) and zoomed on the site (right)

The overall numerical model 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 industrial site itself where the details of buildings and installations have been described and the surrounding area where land use is described i.e. woodland, urban area, rivers etc…). In the second area, only a few large buildings at the vicinity of the industrial site have been explicitly modeled. In the remainder of this area, the influence of surface roughness on flow pattern is treated through a roughness coefficient derived from topographic maps and data collected on site. All natural elements (altitudes, woodland, rivers ...) and all types of facilities that could interact with air displacement have been identified from GIS data (from French Geographical Institute IGN). The numerical representation of the site and its surrounding are shown in Figure 1.

The mesh was optimized to ensure correct numerical resolution of transport and diffusion equations. The mesh is both unstructured and structured with cell sizes ranging from 1m to 150 m. The total number of cells is 1.6 10^6 for a domain height of 300m.

RESULTS AND COMPARISON

Test case 1

The first test case is described in the Figure 2. The red pin shows the location of source 1 while the yellow pins pinpoint the location of the various sensors. The sensors have been positioned according to 2 lines perpendicular to what was assumed to be the wind direction at the moment of the test. The weather conditions during the duration of the test are shown in the table 2. The wind directions covered a 90°sector from 323°N to 49°N in 17 minutes which showed an extremely variable wind. Each wind sector reported in the Table was computed by the software and the numerical cloud was dispersed sequentially on each of the windfields obtained. The expected concentration in sampling bags is calculated by averaging the simulated concentrations field over the sampling time at the location of the sampling system.

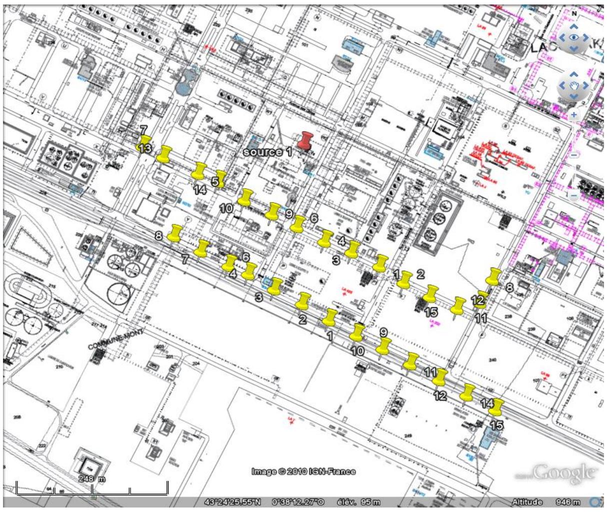

Figure 2. Location of source (red) and sensors (yellow) for test case 1

Table 4. Wind conditions during the experimental release

Duration	Wind speed (m/s)	Direction (°N)
13:30:00.046	3.03	346.5
13:31:00.078	2.25	329.7
13:31:59.703	2.43	323.2
13:33:00.125	2.79	351.0
13:33:59.843	1.77	353.7
13:35:00.078	1.80	42.0
13:35:59.796	1.84	49.3
13:37:00.125	2.64	43.8
13:38:00.046	2.20	11.0
13:39:00.078	2.71	27.5
13:40:00.109	3.09	39.2
13:40:59.921	3.65	40.6
13:42:00.046	3.25	39.9
13:42:59.781	3.17	44.3
13:44:00.109	2.19	11.8
13:45:00.031	0.77	352.9
13:45:59.953	0.66	343.4
13:47:00.078	1.90	36.5

The results obtained both numerically and experimentally are showed in the graphs in figure 3

On Figure 3, the numerical results compare quite well with experimental measurements at two times of sampling (13:30 and 13:40). Both numerically and experimentally, the maximum concentration is found on the same monitor point with a small shift of the plume sidewise probably due to the rapidly shifting wind directions. It can be noted that the maximum amplitude of the concentrations may be missed altogether for some monitoring points experimentally and numerically, since the curves show a flat section on their top.

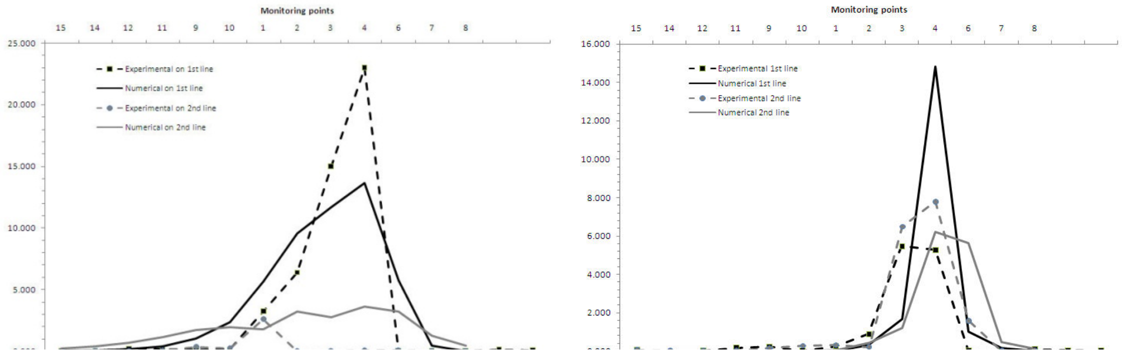

Figure 3. Comparison of measured and simulations concentrations for the 1st and 2nd line of sensors at 13:30 (left) and 13:40 (right)

Test case 2

A second test case is provided here to show the influence of processes at work on the site on the dispersion of the plume. On this test case, cooling towers were located between the point of release (red pin in Figure 4) and the 2nd line of monitoring points (yellow pins in Figure 4).

Figure 4. Set-up of the second test case (left) with emphasis on the cooling towers (right)

The air enters the cooling towers from the bottom at a mean velocity of 4m/s and is ejected from the top at a velocity of 11 m/s and a height of 15 m (Figure 5).

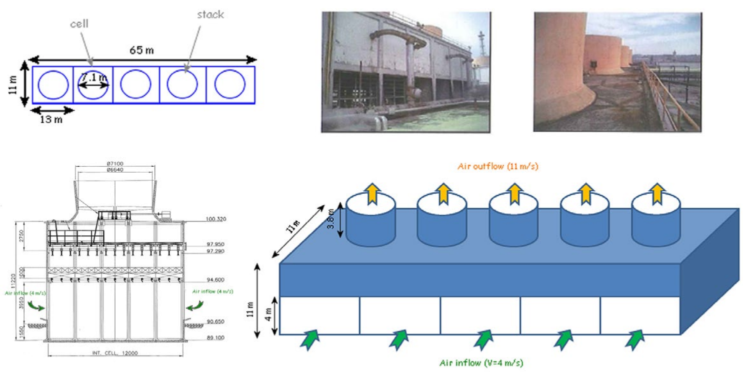

Figure 5. Details of the cooling towers

In order to be able to reproduce the experimentally measured data, the simulation has to take into account this source of momentum. The following figures present the impact of the cooling towers on the local wind field (Figure 6) and on the dispersion pattern (Figure 7).

The concentrations were then checked at three different times (14:00, 14:09 and 14:18) corresponding to the times at which the samplings were recorded. Figure 8 shows a good agreement between the numerical and the experimental results.

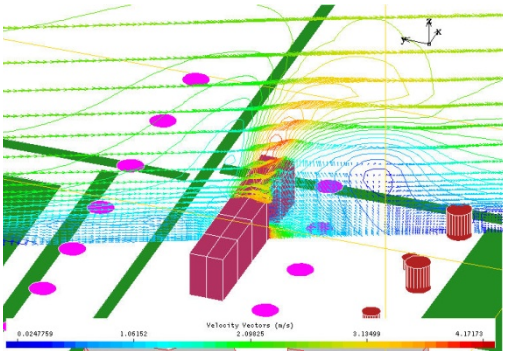

Figure 6. Velocity vectors on a section through the cooling towers

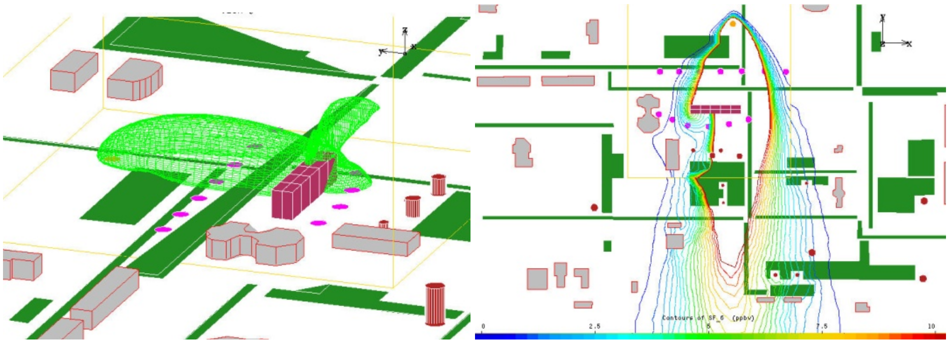

Figure 7. Dispersion plume in isometric view (left) and on a horizontal plane on the ground (right)

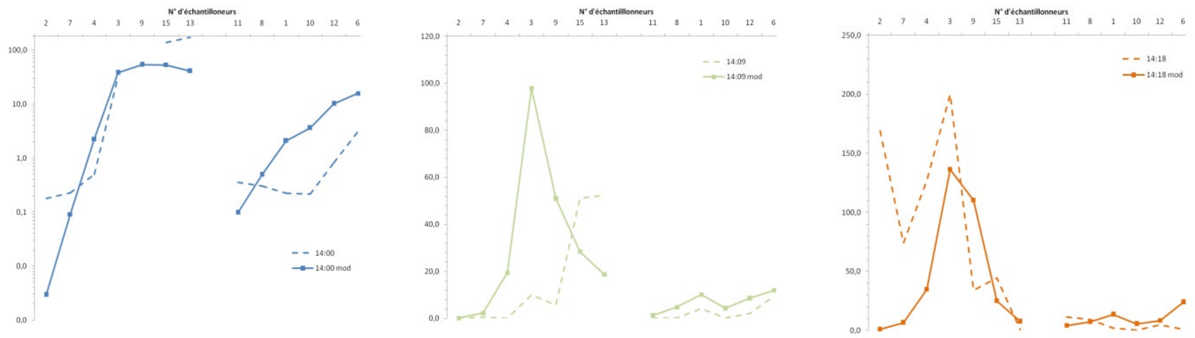

Figure 8. Comparison of experimental data with numerical results for 3 time periods and the 2 sensor lines

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