

## COMPUTING ATMOSPHERIC DISPERSION NEAR BUILDINGS FOR EXPLOSION IMPACT ASSESSMENT

Marie Fabre<sup>1</sup>, Bruno Lequime<sup>1</sup>, Bruno Abart<sup>2</sup>, Erwan Corfa<sup>2</sup>, Armand Albergel<sup>2</sup>  
<sup>1</sup>TECHNIP Paris-La-Défense FRANCE

<sup>2</sup>ARIA Technologies SA, 17 Route de la Reine, 92517 Boulogne-Billancourt FRANCE  
(contact : <mailto:afresneau@aria.fr> [aalbergel@aria.fr](mailto:aalbergel@aria.fr))

### INTRODUCTION

The impact of an explosion following a release from a liquefied hydrocarbon (here butane) storage is quite complex in many levels:

- (1) Source term evaluation including the cold expansion and flashing, and formation of aerosol droplets
- (2) Atmospheric dispersion of two phases (liquid aerosol and gas) taking into account aerosol vaporisation and buildings ('standard' buildings and open building (open shed) in our case)
- (3) Estimation of the explosion severity and over-pressure.

In this presentation, we shall focus mainly on the atmospheric dispersion stage using the MERCURE software developed by Electricité de France but we shall also describe in details the input and the output of the model. The storage is located close to the coast, in a LPG and liquid HC storage facility.

### MERCURE SOFTWARE

MERCURE models atmospheric conditions (modeling of air flow, turbulence and atmospheric dispersion) on the small scale in industrial and urban environment for microscale meteorological studies, as well as the impact of continuous or accidental emissions by taking into account detailed data on obstacles (buildings, topography...).

MERCURE is an atmospheric version of the ESTET ("Ensemble de Simulations Tridimensionnelles d'Écoulements Turbulents") model specifically developed for calculations of atmospheric flow. ESTET solves the Navier-Stokes equations – for average quantities if the flow is turbulent – by the fractional step method in Finite Differences and Finite Volumes, in two- or three-dimensional domains, in transient or permanent equations. We can notice that in the new version ESTET is replaced by SATURNE, the new non-structured CFD of EDF. MERCURE-ESTET was used in this study.

The source term is computed with PHAST software from DNV giving the main thermodynamical parameters of the high momentum jet (velocity and temperature) and also the flow rate in the gaseous phase and in the liquid phase (aerosol), and for some accidental releases scenarios, the effect on source term of impingement of the jet on ground or obstacles.

The last part of the presentation will emphasize on the use of 3D visualisation to understand the heavy gas behaviour near the release. Then we will detail the exploitation of the results of the dispersion phase, as needed for the explosion overpressure computation and the definition of the safety zones.

### SITE MODELING

Generally, it is not necessary to model the whole facilities of a site to simulate the impact of a meteorological scenario on specific buildings. Indeed, the most important when carrying out

numerical simulations at local scale, is to accurately define the main obstacles that may influence the airflow over the site. This generally means that the main buildings and the topography of the site should be taken into account as shown on figure 1 and 2. In this case, the scope of the study is to identify the effect of :

Sea – Land transition (with topography)

The effect of the storage bunkers 1 et 2

The effect of the gas dispatching zone that is a semi-confined building (worst for explosion).

The geometry of the site have been simplified, in order to deal with a limited number of cells and obtain a reasonable CPU time on standard workstations. Working on a simpler geometry enables to treat eventually several cases and scenarios in shorter times. The numerical modelling of the facilities has been realized using information supplied by the main plant layout model. The plan layout model have been simplified in order to consider the main buildings (Autocad DXF numerical file format),

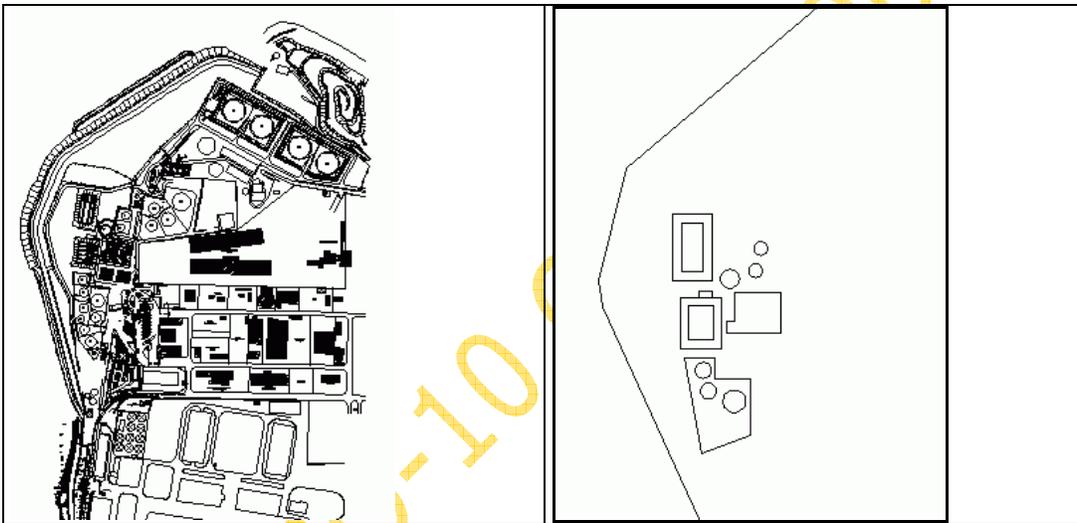


Fig. 4 and 2 ; The real site and the “most influent” buildings

### MESH GRIDS

The mesh generation is often considered as the most important part of the work in numerical simulation. The simulation results are strongly linked to the mesh quality. The mesh generation is always a compromise between calculation time and precision desired.

Considering the meteorological conditions (winds from sea figure 3, and from Land figure 3), we have defined two different meshes. The total domains are about 400m x 300m x 200m. As usual we try to refine the mesh where the gradient are high i.e. near the sources. This mesh generation gives around 300 000 cells.

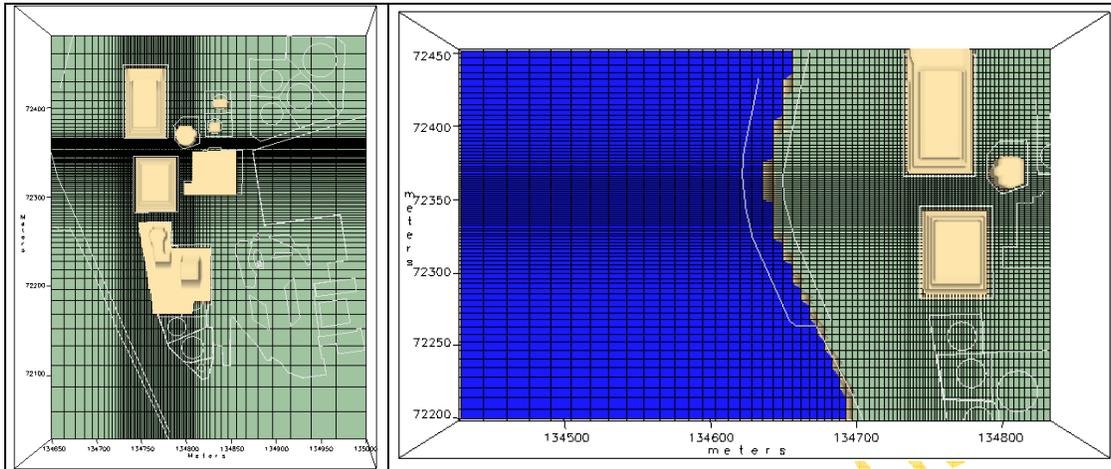


Fig. 3 and 4 ; Horizontal grids respectively for sea winds and for land winds

### METEOROLOGICAL CONDITIONS

The meteorological profiles have been defined as boundary conditions. The profiles are determined from a set of parameters, described as follows:

- Wind direction (mainly toward sensitive zones, as truck and car parks – south east of the domain- etc...),
- Wind speed (mainly 2m/s as “worst” cases and 5m/s as the frequent case, a 0,1m/s wind was also considered as a calm wind),
- Ambient temperature (in this case 20°C and 30°C)
- Atmospheric stability (expressed as an temperature gradient)
- Humidity (used in the aerosols algorithm)

In fact 6 different meteorological profiles were used

### SOURCE TERM

The needed parameters of the sources terms are the localisation of the sources, the main features of the release (jet dimension and orientation, speed and temperature) and the nature of the pollutant (here it is liquid butane -  $C_4H_{10}$ ).

In our case, we had to consider:

- (1) Thermodynamic Flash or direct evaporation following the quick depressurization of the tank,
- (2) The presence of an aerosol phase as droplet with very small diameters,
- (3) The evaporation of the puddle depending of heat transfer between the liquid phase, the soil and the atmosphere.

The source terms are designed considering three scenarios of accident :

- (1) total breaking of the pipe going out the storage bunker considering all the liquid phase as aerosols
- (2) total breaking of the pipe going out the storage bunker considering all the liquid phase as a puddle with slower evaporation rate
- (3) same but on the other storage bunker

The evaporation of the puddle is given as a function of time. Taking into account aerosols is more complex. Inside a complete Navier-stokes equation solver adapted to atmospheric flow (MERCURE), the two phase model described by Rodean and Chan (1986) is used. This

model is based on the “local and instantaneous” equilibrium of all the components locally present (humidity, gas, aerosol). Depending of the vapour partial pressure (vs. the saturation pressure), a part of the aerosol will be vaporized (or condensed) with a decrease (or increase) of the local temperature. This phenomenon and the flow computation is coupled. Humidity is not really negligible due to the vicinity of the sea.

### HAZARDEOUS THRESHOLDS

We define the explosive volume (or mass) as the volume (or mass) of gas inside the two 3D isosurfaces :

- (1) Lower Expl. Limit : 15 000 ppm
- (2) Upper Expl. Limit : 90 000 ppm

### MAIN RESULTS

We can notice a very large spectrum of results due to scenarios definitions and meteorological profiles. We want to present here the difference of result in regard of the explosive volume of butane considering all the liquid phase as aerosol (“free jet”) or the liquid phase is a puddle with its own evaporation timing.

The figure 5 shows on the same plot the explosive volume considering the two different assumptions for the liquid phase ( the same meteorological conditions : 2F Sea Winds)

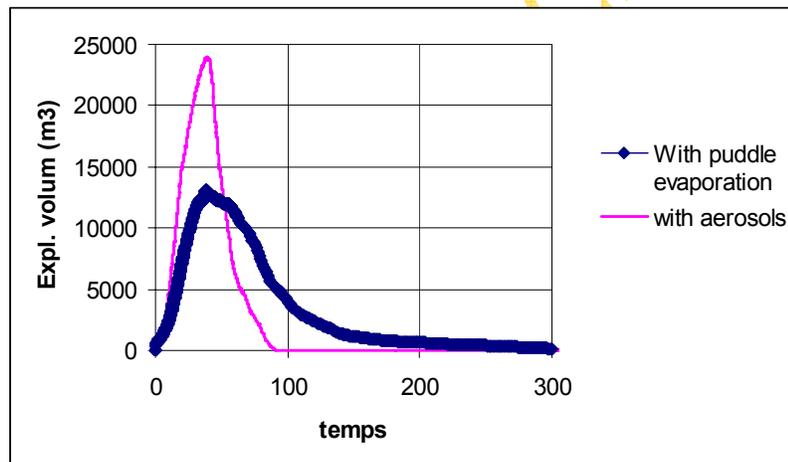


Fig. 5: expl. Volume considering (a) puddle evaporation (b) the liquid phase as aerosol

### CONCLUSION

Beyond comparing CFD model results with those of the PHAST package integral dispersion model UDM, butane cloud flammable envelope and explosive mass content are used to evaluate vapour cloud explosion potential effects. The TNO multi-energy deflagration model is used for predicting overpressure levels and potential damages around congested zones of the site that are reached by butane clouds.

In any case, these computations clearly indicate the impact of the emission scenario and the way how the liquid phase is taken into account.