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LARGE-EDDY SIMULATION OF WIND FLOWS AND COMPARISONS WITH VERY-NEAR FIELD CAMPAIGN DATA

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Abstract

Pollutant dispersion in stable atmospheric conditions is still a phenomenon that is highly difficult to model or to reproduce in an experimental wind tunnel. However, such conditions are of major interest in the field of risk assessment because they are generally conservative and the low level of turbulence induces the most important distance for toxic impact. Using LES approach appears relevant and promising to overcome difficulties related to stable conditions modelling.

The objective of this paper is to present the preliminary results obtained in terms of wind flow modelling with the open source CFD code FDS, from NIST, which is based on Large Eddy Simulation approach. It is essential to determine the best parameterization of this type of code for atmospheric gas dispersion modelling. Starting from atmospheric flow conditions that were observed during INERIS experimental campaign of ammonia release, the process related to satisfy this requirement will be presented.

Key words: CFD LES modelling, experimental data, inlet CFD modelling, stable conditions

INTRODUCTION

Regarding the required citizen protection against industrial hazards, it is nowadays required to be able predicting consequences of the different potential dangerous phenomena that can occur, fire, explosion and dispersion. In this context, if fire and explosion can be destructive, atmospheric dispersion of toxic gas modelling is a key issue mainly because of the large distances generated by such phenomena and the economical consequences required for citizen protection. This point will clearly appear as crucial later in this work in the sense that longest distance corresponds to stable atmospheric conditions.

Gaussian and integral models were developed 40 years ago (Van Ulden, 1974) and are still used for prediction. It is clear however that CFD modelling can be an improvement for being more predictive specifically when natural or anthropogenic obstructions are located in the cloud. RANS approaches should appear as the simplest way. But, on top of specific modifications required for taking into account phenomena as thermal stratification effect on turbulence (Kurbatskii, 2013), such an approach is not able to model the real atmospheric boundary layer considering the specific turbulence intermittency and anisotropy of such a flow. Using LES then appear as the most relevant because of its ability to consider these characteristics by construction. Turbulence anisotropy is due to large scales that are explicitly solved in the LES approach. To go any further, this paper focuses on the ability of the FDS code to model such a phenomena. Considering the importance of dispersion in stable conditions as mentioned above in this introduction, stable conditions are mainly considered for modelling.

Two steps are required for such an objective. The first is to demonstrate the ability of the FDS code to be reproductive, the second is to build a methodology for being predictive. This paper clearly focuses on the ability of the CFD code to be reproductive that means to show the possibility of modelling a given experiment. One of the main difficulties to do this is the need of detailed and reliable input data, considering using LES for atmospheric dispersion modelling requires building turbulence spectrum. Large scale INERIS ammonia releases were used in this paper mainly because it corresponds to a free field jet release that can be confronted to CFD to check the ability of these tools in predicting the consequences of toxic industrial chemicals (TIC s) atmospheric dispersion following an accident. The main part of the paper details the methodology built for evaluating the FDS capability to model such an experiment. Available methods and its application to SIRTA experiment are proposed in the perspectives presented in this paper.

DEMONSTRATION OF THE FDS CAPABILITY TO BE REPRODUCTIVE

FDS for “Fire Dynamics Simulator”, is a CFD freely available code developed by NIST (McGrattan, 2005) to compute fires and smoke propagations. Turbulence model is based on the Large Eddy Simulations (LES) approach. Previously some LES simulations were published by Mouilleau et al. (Mouilleau et al., 2008) based on a simple approach uncorrelated with experimental measurement or theoretical development. Such an approach enables to build a fluctuating velocity profile in the domain inlet. The simple approach developed in this work is an extension of this methodology to take into account the large variety of frequencies due to the large number of turbulent fluctuations. This approach is based on a Fourier analysis of an experimental profile.

Ammonia dispersion INERIS field tests

Ammonia dispersion field tests performed by INERIS (Bouet, 1999) are briefly presented. In 1996–1997, INERIS conducted real-scale releases of ammonia in open air with the help of major sponsors. These tests were intended to reproduce as closely as possible an accidental scenario that may occur in a real industrial facility. Outdoor experiments were conducted on the testing site of CEA-CESTA (Centre of Scientific and Technical Studies of Aquitaine) that had a surface area of 950 ha and was completely flat. **Figure 10** shows the whole measurement area in CEA-CESTA field.

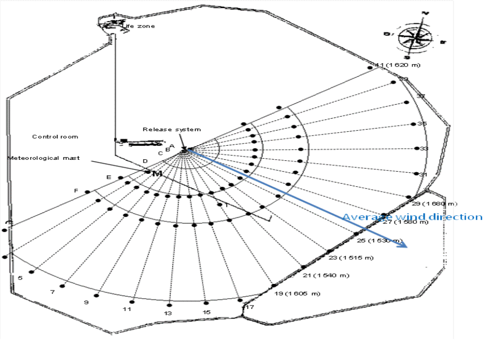


Figure 10: The whole measurement area in CEA-CESTA for the ammonia experimental test cases; sensor arcs locations (distances from the release system : 20 m, 50 m, 100 m, 200 m, 500 m, 800 m and 1700 m for corresponding referenced letters A, B, C , D, E, F, G)

During the experiments, the atmospheric conditions were determined using a meteorological mast which was installed 350 m from the release point (label “M” in **Figure 10**). This mast was 10 m high and was equipped with 3 cup anemometers located at 1.5, 4 and 7 m above the ground, a wind vane at 7 m and an ultrasonic anemometer at 10 m. A weather station was also installed near the testing site. It allowed recording the ambient temperature, the relative humidity and the solar flux at a height of 1.5 m. For all apparatus, the scanning frequency was set to 1 Hz except the ultrasonic anemometer whose frequency was adjusted to 10 Hz. Catalytic sensors (near field) and electrochemical cells (far field) allow to measure ammonia concentration. Sensors were positioned in 7 arc shapes centered on the release point (see **Figure 10**).

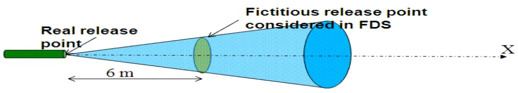
Several tests release cases were conducted with mass flow rate up to 4 kg/s. For the scope of the present study the trial case 4 is considered. It corresponds to a free field jet release. As expected, the ammonia cloud behaved like a heavy gas and no elevation of the cloud was observed. For a relative humidity of 82%, the visible cloud length was about 500 m. This visibility is associated with the condensation of water contained in the ambient air once this latter is entrained into the two-phase release. During these tests, it was found that the temperature of such release can drop down to -70°C. Once the cloud is sufficiently heated by dilution with ambient air, the cloud is no longer visible. The meteorological condition is sum up in the **Table 5**.

Table 5. sum up of atmospheric conditions for trial case 4

Ambient temperature	Relative Humidity	Solar Flux (kW/m^2)	wind speed (m/s) at 7 m	Pasquill Class
12.5°C	82%	0.25	2.7	D

Implementation of a biphasic and dense gas term source

FDS software can not directly deal with multi-phase releases. In order to bypass this limitation, a simple methodology has been developed to achieve an equivalent term source. Papadourakis et al. (1993) approach was previously used for computing source term. It is then implemented as an equivalent term source in FDS simulation. A brief summary of this latter is given in **Figure 11**.



Jet characteristics at X = 6 m
Axis jet velocity: 25 m/s
Vapor Temp: -50 °C
Liquid mass fraction: 0.5
Section area : ~1 m²
Concentration of NH_3: 0.11
Concentration of air: 0.82
NH_3 Mass flow rate : 4.2 kg/s (experimental data)
Air mass flow rate: 19.1 kg/s
Total mass flow rate = 23.3 kg/s

Figure 11: description of the term source implemented in FDS simulation

Adaptation of an experimental signal for an input LES

Previous CFD flow simulations with RANS approach show that better results are obtained when the inlet conditions are fitted to measurements both for mean velocity profile or for inflow turbulence (Milliez and Carissimo , 2006; Milliez and Carissimo, 2007). Preliminary tests with FDS with mean velocity profile at inlet of the flow show that turbulence is not sufficiently generated inside the computational domain. This result is consistent with the physics of the LES model that considerer instantaneous velocities for each component U, V and W. Within the context of this current experimental validation approach we intend to reproduce the experimental signal. In LES, the inlet condition is a definition of mean velocity and its temporal fluctuations. A power law is used to fit the mean wind module along the experimental vertical profile (1.5, 4 and 7 m). The wind velocity signal in time for FDS inlet boundary condition is obtained by performing a Fourier analysis in time on the experimental signal (reference point : 7 m on the mast). It allowed building the fluctuating wind velocity signal for the U and V components. The construction was performed by using an orthogonal transformation. The signal is then built on the basis of linear sum of cosine and sine functions (equation (1)) with coefficients representing the energy contained in each mode (k).

$$u' = \sum_{k=1}^{n} a_k \cos(2\pi \cdot f_k \cdot t) + b_k \sin(2\pi \cdot f_k \cdot t) \qquad (1)$$

In the numerical simulation, the 50 most significant coefficients were introduced in the inlet profile to reproduce U and V signal components in time. The coefficients are directly proportional to the turbulence intensity such that we ensure to introduce most of the turbulence information. Due to the lack of data along vertical axis, the fluctuant component of the velocity profile is taken proportional to the one at 7m and weighted by the mean velocity along the main wind direction. Therefore the turbulence intensity is constant along the vertical profile. This constitutes a strong hypothesis to characterise the inlet flow turbulence, however it seems less significant in the specific case of massive release located close to the ground. In summary, the 2D inlet boundary is set up by a homogeneous wind in space with no vertical component (W= 0 for all z). In this condition free divergence is satisfied. This approach corresponds to the simplest effective approach (Tabor et al., 2010) to synthesize the inlet conditions for large eddy simulation. This approach is similar of Kondo et al. (1997) approach, and developed by Shirani et al. (1981). **Figure 12** presents the computational domain used in the calculations performed in the present study. Dimensions, source release location and boundary conditions are the main features shown. The calculation domain is defined by a single right parallelepiped mesh. This computational domain is 1000 m long with a grid cell size of 0.5 m in the near field of the release and of 1 m in the far field. Lateral and outlet boundaries are open boundaries. The ground is no-slip walls. The upper boundary is a mirror condition, i.e a free-slip wall.

Simulations of the flow were performed before dispersion modelling of the release. A physical time of 1000 s is sufficient for FDS to generate a stabilized turbulence along the whole domain. The unsteady simulations were performed with a time step size automatically estimated according to the CFL requirement.

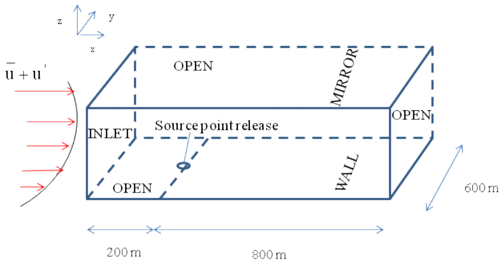


Figure 12: computational domain

The Smagorinsky model was used for the LES computation. The value of the Smagorinsky constant C_s was 0.2. The time discretization is based on an explicit predictor-corrector scheme, that is first order accurate in space and time such it ensures numerical stability. The second order scheme would be more accurate and is being tested. Simulations of the atmospheric flow without release were performed in order to observe the evolution of the spectra between the inlet and the outlet boundary. It shows a good conservation of spectra energy for the large scale spectral energy (**Figure** 13). However, a part of the energy has moved from the large to the small structures. This result is consistent with LES approach that aims to solve mainly the energy-containing motions.

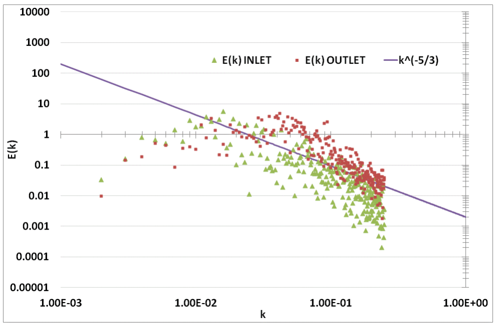


Figure 13: comparison of the turbulent energy spectrum at the inlet and outlet conditions

Summary of the atmospheric dispersion results

The results of the ammonia release modeling obtained with the modeled atmospheric flow described in the previous section are briefly presented below. A roughly comparison between modeling results and experimental observations shows that whole shape of the modeled cloud is in good accordance with experimental observations (see **Figure 14**). The modeled cloud of ammonia behaves well as a dense gas around several hundred meters.

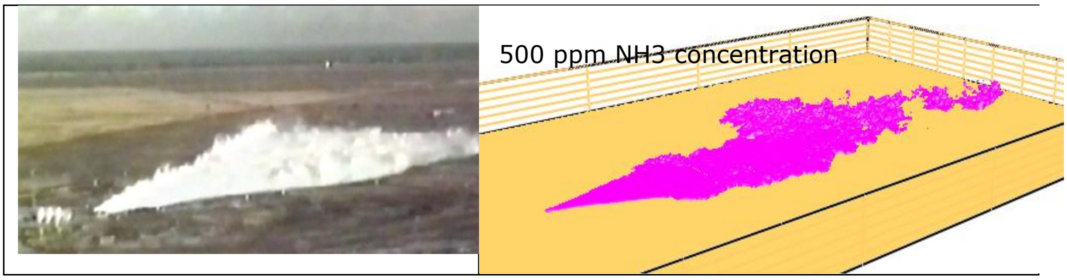


Figure 14: comparison between the overall form of the experimental cloud shape and simulation results

Figure 15 shows comparison between simulation results and experimental data for the whole set of receptors. Comparisons are performed with mean concentration. The averaging time roughly corresponds to the exposition time period defined by arrival time and departure time of the cloud. Taken into account uncertainty on sensors measurement, it could be estimated that the modelling results compared in a good accordance with sensor measurements.

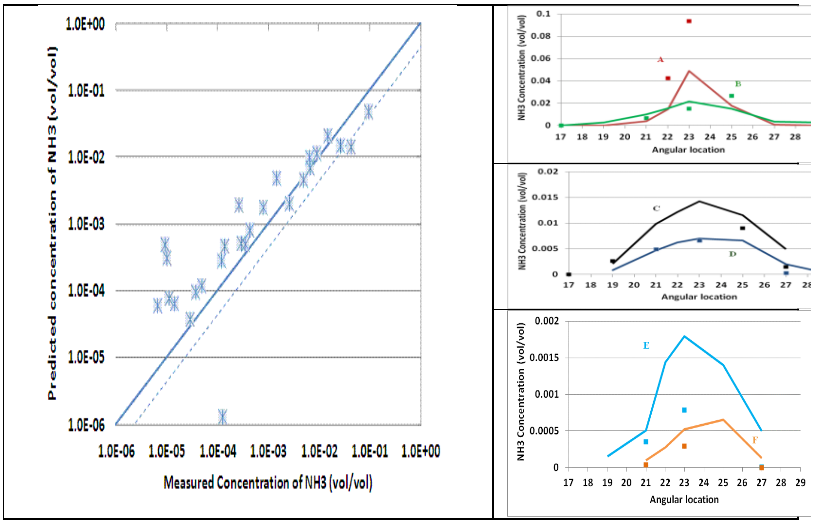


Figure 15: Comparison between simulation results and experimental data for the whole set of receptors (logarithm scale)(left graph) and for each arc (A, B, C, D, E ,F) of receptors (right graphs)

These promising results by LES approach are interesting regarding the complexity to describe both the release in the near field and the far field. The FDS code allows modelling the strong cooling effect of the release. The necessity to set up a representative energy spectrum in the context of LES modelling has been done in this experimental comparison.

TOWARDS PREDICTIVE MODELING FOR STABLE CONDITIONS

An overwhelming variety of method (recycling method, synthetic method, forcing method) aiming to generate inflow boundary conditions for LES (Jarrin et al., 2008) have been reviewed in the literature. The method of inlet generation for LES approach, presented in this paper, appears as very simple. To go further it is worth using methods that introduce turbulence in space as well as in time. These methods are based on more statistical information of the flow turbulence. To reach this objective we propose to use experimental velocity data from SIRTA experiment that allow providing (Wei et al., 2014) significant information on space and time correlation of the wind flow in case of atmospheric stable conditions. In order to harmonize the inlet flow between definitions usually assessed by Gaussian model or RANS modelling, the authors suggest to establish a link with turbulence characteristic used by more classical models or theoretical atmospheric classification as the one of Pasquill.

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