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HARMONIZATION IN CFD APPROACHES TO ASSESS TOXIC CONSEQUENCES OF AMMONIA RELEASES

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Abstract: In the framework of land use planning, massive releases have to be modelled considering they generate important toxic effect distances. The common way to deal with such scenarios is currently based on Gaussian models or, more recently, CFD codes based on a RANS turbulence model. While the first does not enable taking account of the environment with a high level of precision, the second are not suitable for accounting for Atmospheric Boundary Layers (ABLs) anisotropy. Using LES CFD approaches then appears nowadays as promising to overcome those difficulties. However it is necessary to perform the best input parametrization among a large variety of method (recycling method, synthetic method, forcing method) to generate appropriate inflow boundary conditions. The objective of this paper is to present results obtained with the open source LES CFD code FDS by using synthetic eddy method. Parameterizations to generate inlet conditions were tested and compared to large scale INERIS ammonia releases. Comparison with the RANS CFD model *Code_Saturne* and the shallow layer SLAB model are also presented and discussed.

***Key words**: CFD LES modelling, experimental data, inlet CFD modelling, ammonia release*

INTRODUCTION

Several models are used in the framework of land use planning, based on a large variety of nature and complexity. For an identical accidental release in the atmospheric, within the context of a regulatory study, discrepancies could appear in terms of computed distances, this means major differences in impacted zones. Those variations can be observed either between atmospheric CFD model results or with conventional approaches as Gaussian or shallow layer approach models. Reasons that can explain these discrepancies are numerous and have various origin. A major issue for risk assessments is the harmonisation of input data for the flow modelling between widely-used approach and CFD (RANS or LES) approaches which using is continuously increasing. These latter can be an improvement for being more predictive specifically when natural or anthropogenic obstructions are located in the vicinity of the release. RANS approaches appear as the simplest way but some limitations can appear considering the specific turbulence intermittency and anisotropy of the flow of the ABLs. LES modelling appears then as relevant because of its ability to consider unsteady and anisotropic turbulence and its consequences on the cloud dispersion.

This paper focuses on the ability of the shallow layer SLAB, the RANS code (*Code_Saturne*) and the LES code (FDS) to model an ammonia release experiment and the work required to harmonize input data for predictive atmospheric model. Large scale INERIS ammonia releases were used in this paper because it corresponds to a free field jet release that can be compared to atmospheric dispersion model to check the ability of these tools in predicting the consequences of toxic industrial chemicals (TIC s) atmospheric dispersion following an accident. Comparisons between modeling results from these three approaches and experimental measurement are presented and analyzed.

EXPERIMENTAL TEST DESCRIPTION

Ammonia dispersion field tests performed by INERIS were presented in a previous paper (Bouet, 2005). INERIS conducted real-scale releases of ammonia on the 950 ha flat testing site of CEA-CESTA (Centre of Scientific and Technical Studies of Aquitaine). During experiments, the atmospheric conditions were analyzed using a meteorological mast. 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 1.5 m above the ground. Sensors were located in 7 arc shapes centered on the release point. Several release test cases were achieved with mass flow rate up to 4.2 kg/s. For the scope of the present study the trial case 4 is considered (release duration time: 10 min) which corresponds to a free field jet release. As expected, the ammonia cloud behaved like a heavy gas. A description of this experimental trial and a modeling study have already been presented in a previous paper (Lacome et al., 2014). In this present paper an enhanced wind flow analysis is carried out to take into account additional measurements provided by ultrasonic anemometer (see **Table 1**).

Table 1. Ultrasonic anemometer (10 Hz) measurements (over first 5 mins of the release) for trial case 4

Ambient temperature	**LMO (-)**	**u_* (m/s)**	**wind speed (m/s) at 10 m**
14.82°C	-166	0.36	3.24

GOVERNING EQUATIONS FOR THE 3 MODELLING APPROACHES

The widely-used dense gas dispersion SLAB has been used to simulate the trial case. It is available for free thanks to the Environmental Protection Agency (EPA). The RANS CFD simulations were performed with *Code_Saturne* (CFD freely available code), which has been previously tested on flat terrain (E. Demael and B. Carissimo, 2008) and obstructed environment (M. Milliez and B. Carissimo, 2007). The LES CFD runs were achieved with FDS a freely available CFD code provided by the NIST (McGrattan, 2005) and initially dedicated to fires and smoke propagations modelling. The main features of the 3 modelling approaches are briefly summarized in the following part.

SLAB

The model can handle horizontal jets (Ermak, 1990); in the far field a shallow-layer approach is widely used to disperse a dense gas (Hanna et al., 2008) according to the observed behavior of the release.

RANS

The governing equations are solved under Boussinesq's hypothesis. Simulations were run with an adapted $k - \varepsilon$ turbulence model for atmospheric flows (Wei, 2016). The transport equations for the turbulent kinetic energy k and the scalar dissipation rate, ε, take into account the wind shear and buoyance effect on production or dissipation of k. This latter term is formulated by means of potential temperature gradient. Indeed, transport equation for the potential temperature, θ, profile is solved along the domain. The models constants for $k - \varepsilon$ turbulence model take the values modified for atmospheric flows following (Detering, 1985) where $C_\mu = 0.03$ according to the work of Duynkerke (Duynkerke, 1988) and the value of $C_{\varepsilon 3}$ is taken after (Violet, 1988): $C_{\varepsilon 3} = 0$ for a stably stratified atmosphere and $C_{\varepsilon 3} = 1$ for an unstably stratified atmosphere corresponding to the present studied case.

LES

Turbulence model is based on the Large Eddy Simulations (LES) approach. The fundamental idea of LES is the segregation between large scales, that are explicitly solved, and small ones, that are modelled. Because the anisotropy is governed by the large scale and considering small scales are dissipative ones, this consequently enables solving the whole characteristics of turbulence in the ABLs. The key issue then consists in prescribing relevant velocity profile in terms of instantaneous velocity. In the last version of FDS, v6.1.2, was introduced the SEM methods as developed by Jarin (Jarin et al. 2008).

ADAPTATION OF AN EXPERIMENTAL SIGNAL FOR THE CODES INFLOW

SLAB

The model was run with the optimum source release terms knowing the experimental mass flow rate and that experimental observations showed very little rainout deposition on the ground. The flow input is set by choosing a stability Pasquill class of type C, according to the sonic anemometer measurements, and a roughness value of $z_0 = 0.03$ m was selected according to the land cover of the experimental site ground (prairie grass). An enhanced study, based on a statically wider wind study of the site, would be necessary to assess this value that is generally sensitive for atmospheric dispersion modelling.

RANS

The atmospheric stability class is represented by the inflow boundary condition for the velocity, the turbulent kinetic energy k, dissipation of turbulent kinetic energy ε and temperature profile. The inlet and the top boundary are specified by the Dirichlet condition. The outlet is a free outflow condition. The lateral boundaries are symmetry condition. The wind velocity and direction were modelled as constant, i.e. wind-meandering was not modelled. Previous CFD flow simulations (Milliez and Carissimo, 2007) with RANS approach show that better results could be obtained by fitting the inlet conditions to measurements for both the mean velocity profile and the turbulence intensity. According to these previous results, a power law velocity, according to the stability class reported by Barrat (Barrat , 2001), i.e., n = 0.16 (stability class C), is used to build the velocity profile (see **Figure 1**). The turbulent kinetic energy and the dissipation of turbulent energy profiles are built using the similarity functions proposed by Dyer (1974) for unstable condition which main inputs, i.e the friction velocity (u_*) and the Monin-Obukohv length, were measured by anemometer sonic (see **Table 1**). The scalar dissipation rate profile is based on the hypothesis that viscous dissipation balances shear production and buoyancy. The profiles of k, ε and the turbulent viscosity, K_m are specified as follows:

$$k(z) = \frac{u_*^{2}}{\sqrt{C_\mu}}\sqrt{1-\frac{z}{L}} \qquad \varepsilon(z) = \frac{u_*^{3}}{\kappa}\left(1-\frac{16z}{L}\right)^{-1/4}\left(1-\frac{z}{L}\right) \qquad K_m(z) = C_\mu \frac{k^2(z)}{\varepsilon(z)} \tag{1}$$

LES

When using LES, defining a representative turbulent flow field as inflow boundary condition is required. This flow should satisfy prescribed spatial correlations and turbulence characteristics. The method used here is the synthetic eddy method (SEM) (Jarrin and al, 2014). The SEM approach involves the generation and superposition of a large number of random eddies, with some control on their statistical properties and using the following predefined shape function for the velocity fluctuation:

$$u'(x) = \frac{1}{\sqrt{N}}\sum_{k=1}^{N} a_{ij}\varepsilon_j^k f_\sigma\left(x - x^k\right) \tag{2}$$

These eddies are then transported through a 800 m long rectangular cross-section domain. The resultant, time-dependent, flow field taken from a cross-section of this domain can be extracted and imposed as an inlet condition for LES. This method allows the desired Reynolds stress field to be prescribed. Inflow boundaries for synthetic method available in FDS consists of data given by following experimental results: U_{mean} mean velocity, RMS_x Root Mean Square velocity in x-direction matching with mean wind direction, L_x integral scale in x-direction. Inflow mean velocity profile follows an exponential law. Integral length scale may be defined by assuming the advection of turbulent structures by the averaged wind such as: $L_x = U_{mean} T_x$ with T_x : observed integral time scale in x-direction. The atmospheric data used as inflow boundary conditions for LES approach are presented in **Table 2**.

Table 2. Atmospheric input data for LES approach

Anemometer altitude (m)	**Mean velocity U_{mean} (m/s)**	**Integral time scale T_x (s)**	**Integral length scale L_x (m)**	**RMS_x**
1.5	2.59	12	31.0	0.72
4	2.94	14	41.1	0.68
7	3.18	20	63.6	0.64
10	3.24	-	-	0.9

RMS velocity fluctuation set up at inlet is isotropic. In other words, diagonal components of the Reynolds stress are identical and all others are set to 0. The outlet is a free outflow condition. The lateral boundaries are symmetry condition. No temperature profile is set up at the inlet.

The **Hiba! A hivatkozási forrás nem található.** summarizes the data used as inflow boundary condition for the three approaches.

Table 3 : Harmonized input data for the SLAB model, RANS and LES approach

Code	**Dispersion model**	**Common input flow Data**	**Specific input flow data**	**Source term modelling**
SLAB	Shallow layer	Mean velocity profile Ground roughness of 0.03 m	Pasquill Stability class	Orifice release conditions: NH_3 Mass flow rate of 4.2 kg/s, 0.6 liquid fraction
Code_Saturne	RANS		Turbulent kinetic energy and dissipation and temperature profile (not shown) based on experimental friction velocity, LMO and heat flux	Equivalent gas source term located at 6m from orifice NH_3 mass flow rate of 4.2 kg/s Total mass flow rate of 37.5 kg/s Surface area of 1 m²
FDS	LES		Isotropic integral time, length scale and RMS_x based on experimental data	

SOURCE TERM

FDS and *Code_Saturne* cannot directly deal with high speed multi-phase releases. Then in order to bypass this limitation, an equivalent source term (see **Hiba! A hivatkozási forrás nem található.**) was implemented at a distance from orifice, thus leading to moderate velocity and a weak liquid fraction which can be readily handled by CFD codes (see Lacome and al., 2014).

MESH

The modelling area used is 1300 m x 600 m x 60 m in the x, y and z directions, respectively for RANS and 800 m x 400 m x 40 m for LES. The computational grid consists of approximately 1.2 million of hexahedral volume elements for RANS (expanded grid with an expansion ratio lower than 1.2) and 6.5 hexahedral volume elements for LES. The minimal space length is 0.5 m corresponding to cells located close to the ground, it allows implementing the source term with 4 cells.

FLOW ANALYSIS FOR DIFFERENT APPROACHES

The first step in the whole simulation task consists in checking whether the wind flow is correctly modelled or not in order to demonstrate that a homogeneous ABL is obtained along the whole domain. For the RANS approach, the results show that the ABL profiles are well sustained, except for the turbulence kinetic energy which decreases downwind from the inlet. Difficulties faced of in the present atmospheric condition (slightly unstable) were expected and this issue is addressed by previous works (Gorlé, 2009; Batt *et al*. 2016). However, it turns out that turbulent viscosity profile (see Figure 1) are eventually quite well sustained along the domain close to the ground (z < 5 m). Consequently, it is assumed that the difference between ABL profiles at inlet and at outlet generates a weak impact on dispersion predictions. Moreover, the theoretical profile used to build the input turbulence slightly overestimates the value measured by sonic anemometer at 10 m height (see Figure 1) such the level of turbulence modelled by *Code_Saturne* could be deemed close to the one observed during the test.

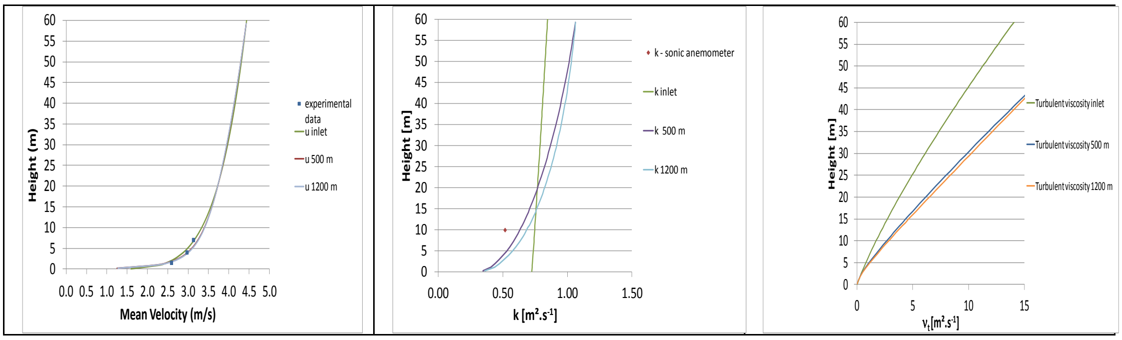

Figure 1. Predicted results for the flow ABL profiles at the inlet (x=-100m), centre and outlet of the domain with RANS CFD code

In Figure 2 flow characteristics obtained with LES approach at different x-positions are compared against inflow conditions and experimental data.

Mean velocity is well maintained in the domain. However, turbulence decreases rapidly in the first part of the domain but RMS profiles are sustained in a steady way. This turbulence decrease was expected (Hanna, 2002) and explained the underestimation of friction velocity when compared to experimental data. A foreseeable solution would consist in stabilizing the flow as a preliminary step in a given domain.

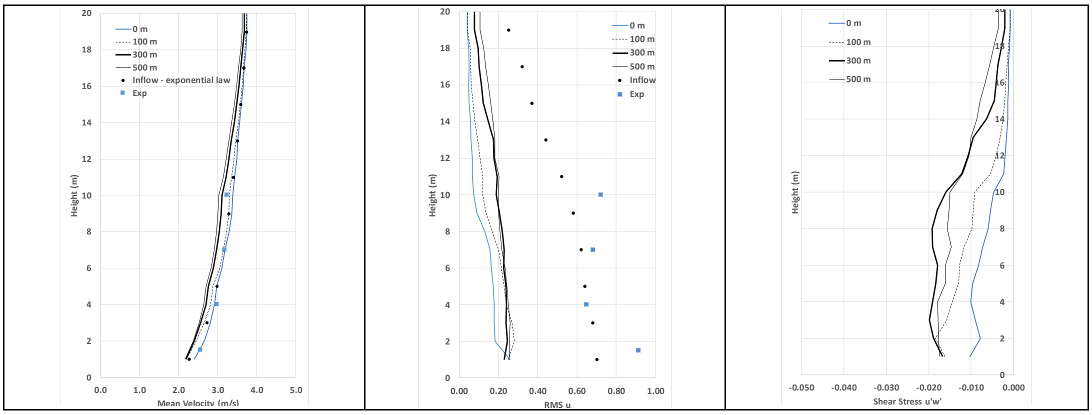

Figure 2. Flow characteristics against inflow conditions (x=-100m) and experimental data - LES approach

ANALYSIS OF THE ATMOSPHERIC DISPERSION RESULTS

Figure 3 and Figure 4 shows comparison between experimental and predicted mean concentrations obtained with the three codes.

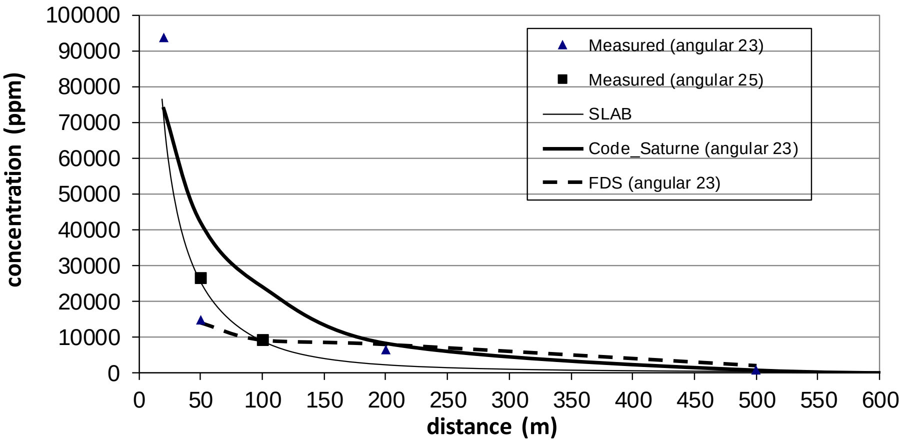

Figure 3: Comparison between simulation results and experimental concentration data along the axis (angular 23 and 25) downwind of the source which are closest to the mean direction of the wind

It can be noticed that numerical results are in good agreement with sensor measurements, although meandering effect has not been taken into account. Previous work (Lacome, 2014) has considered this effect. For RANS and LES approach these results are promising regarding the complexity to describe both the release in the near field and the far field. However, the model slightly over-predicts the measurements respectively in the near field (50 m < x < 200 m) for the RANS model and in the far-field (x > 200 m) for the LES model. An explanation could be the insufficient level of mixing due to the atmospheric flow. Indeed, previous studies (Demael, E. and B. Carissimo, 2008; Hanna, 2002) demonstrated this possible k- ε and LES turbulence model's weakness. Bearing in mind the use of an optimum source term, it can be noticed the good accordance between the concentrations decrease, along the lean wind axis, modelled by SLAB and the observations.

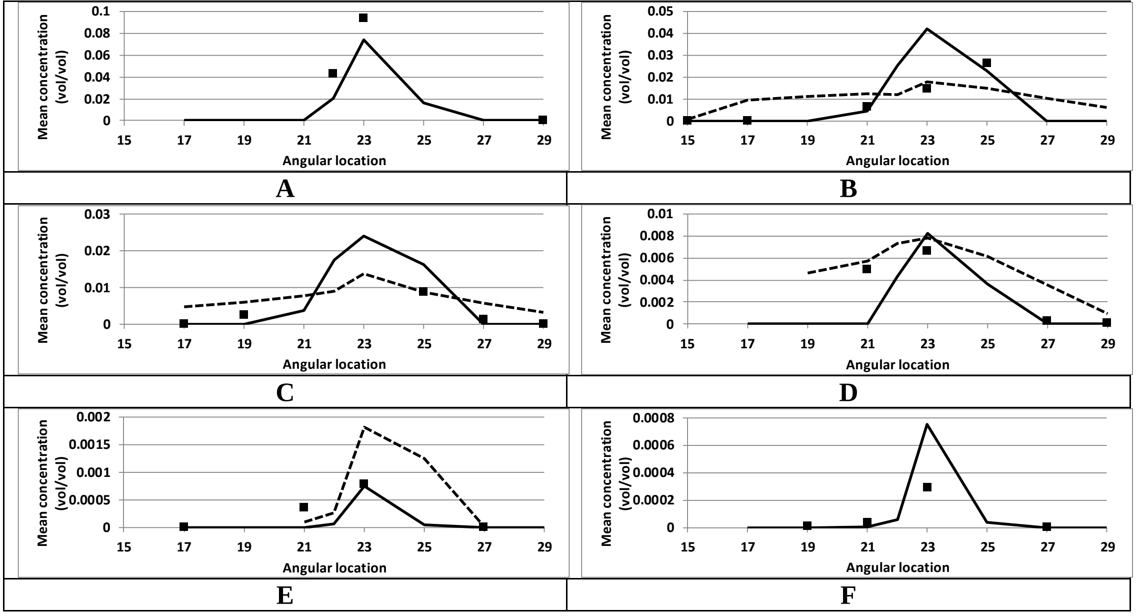

Figure 4. Comparison between simulation results (FDS: dotted line; *Code_Saturne* : continuous line) and experimental concentration for each arc (A=20 m, B=50m, C=100m, D=200m, E=500m, F=800m) of receptors.

CONCLUSION

Several dispersion models of different nature (shallow-layer, RANS, LES) have been used to model a large scale experimental ammonia release. Based on experimental observations analysis, flow input data and source term of different level of complexity have been set up for each approach. While LES code (FDS) need the most advanced input analysis, mean velocity and ground roughness form the common input parameter to the three approaches. The same equivalent gas source term located has been set for LES and RANS approaches in order to harmonize practices. Expected difficulties to maintain the turbulence level along the flat domain have been encountered for CFD approaches. Taking into account the inherent complexity to model and simulate the atmospheric turbulence, predicted concentration is in good agreement with experimental data for both RANS and LES approach.

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