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Dispersion in Confined Building: a Coupled Approach

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Abstract: Modelling gas dispersion in mechanically ventilated building is a challenge for safety engineers. A leak in such an infrastructure can generate two different consequences: toxic effect or blast effect after a flammable vapour cloud ignition. In both case, it is important to be able to predict the gas behaviour using numerical tools in order to be able to design adapted ventilation systems. Gaseous products are generally stored under pressure that induces high velocity in case of release from the tank or following a line rupture. Considering this important pressure, the jet zone is a highly complex zone with a Mach number higher than 1 that induces shock waves. These waves correspond to discontinuity of the flow. After this jet zone, a transition region (air entrainment) is observed and can be characterised by the beginning mixture of the gas with air. This also corresponds to an expansion of the jet diameter inducing a velocity decrease. Finally, after this zone, the flow becomes governed by the ventilation system where the Mach number is lower than 1. To model gas dispersion in closed enclosure, CFD models can be used. Such codes enable to predict the different physical quantities in the whole domain along time. However, most of these codes are not able to model complex phenomena such as ones that characterised the jet region. CFD codes are able to capture such a complex physic require mesh in the jet zone that is not in accordance with the objective to model the whole infrastructure considering current computing limitations. To overcome this and making achievable such modelling, a coupled approach between a 1D jet model and a CFD code is proposed. The 1D model predicts gas behaviour in the jet zone while the CFD code describes the concentration and velocity in the whole domain. The FDS CFD code was used. This code is based on the LES approach for turbulence modelling. Such an approach is highly interesting for safety because it enables not to predict an average configuration but a realistic one. Because of the well known capability of this code for predicting smoke behaviour considering ventilation, it is useful to wonder about its capability to model gas dispersion in buildings. A comparison between FDS, coupled with the 1D model, results and experimental ones are given. The experimental results were obtained in an 80 m^3 room equipped with a ventilation system in which ammoniac was injected. Two different ventilation regimes were used and concentrations were measured in several locations inside the room at different heights. Comparisons between experimental and numerical values shows a great agreement and leads to the conclusion that the FDS code is a pertinent tool for gas dispersion modelling in confined building when coupling this code with a 1D jet model.

Keywords: toxic dispersion; critical infrastructure; large eddy simulation; coupled approach

1 Introduction

Toxic releases in large enclosure are a topic of interest regarding both accidental risk and intentional threat. On the first hand, toxic gases are commonly used in industrial facilities and that can generate, in case of release, catastrophic consequences. Several gases must be considered in such a configuration, ammonia, chlorine, hydrogen cyanide, ... To provide an example, ammonia, which is commonly used for cooling is generally stored at its critical pressure will be at 8 bars. Such a pressure will generate, in case of release, important velocities and the jet can, in some configurations, become sonic.

On the other hand, toxic gases can also be used for terrorism. In such a case, not only industrial chemicals can be used but military ones too. For the first ones, they could be introduced using pressurised containers that induce the same problematic as accidental release. For the second, i.e. the military toxic gases, they are liquid under atmospheric conditions and consequently, they could be release as a pool. This second case is out of the topic of the present paper that focuses on the link between a pressurised gaseous release and the dispersion in a large enclosure.

So, as mentioned above, the objective of this paper consists in modelling a high pressure gaseous release in a large enclosure. This enclosure can be either an industrial building or a critical installation as airport or train station for example. In both cases, dimensions of the domain will be strongly larger than the characteristic of the jet. So, two different zones must consequently be distinguished with own properties to be discussed, Fig.1 and Table 1. As represented on this figure, dimension of the infrastructure can be larger than hundreds meters while the jet characteristic size is of about of cm. Consequently, characteristics dimensionless numbers for the two flows can be highly different. To keep this in mind, summarize characteristic dimensions and dimensionless numbers for a ventilated infrastructure, industrial or critical one, and for the release jet.
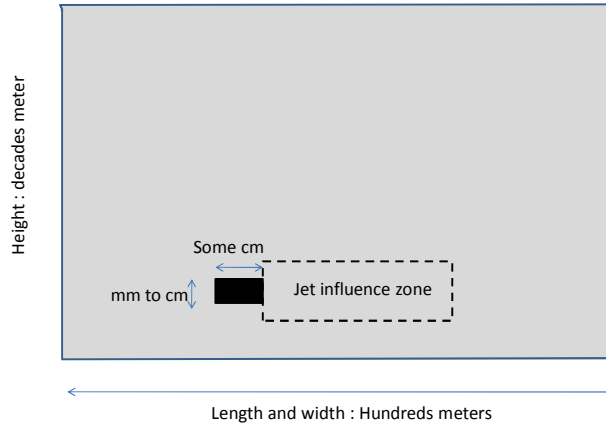
Fig.1　Schematic representation of nested physics

Table 1　Characteristic of the infrastructure and jet

Characteristic	Infrastructure (grey on Fig.1)	Jet (black on Fig.1)
L	Decades to hundreds m	Some mm to cm
U	≈ 1 m/s	> 300 m/s
C	10^2 to 10^6	1 near the hole
Re	1×10^6 to 1×10^7	1×10^4 to 5×10^6
Fr	0.01 to 0.5	5e6 to 15e6
Ma	$\ll 1$	≈ 1 to > 1

Before going any further in the physical requirement, the dimensionless numbers must be clarified. The Reynolds number, $Re=(\rho UL)/\mu$, represents the ratio between inertia and viscous effects and is characteristics of the turbulence. Higher is the Reynolds more important the turbulence is. It appears that, even if the velocity, and consequently the shear, are lower in the infrastructure without the jet, characteristic dimensions of the room governs because this allows a large range of possible turbulent scales. Consequently, it should be considered that turbulent phenomena are mainly attached to the ventilated infrastructure. The Froude number, $Fr=U^2/(gL)$, represents the relative effects of velocity induced forces and gravity ones. It appears clearly that, for the present case, the jet flow is governs by velocity forces in the near field. The Mach number, $Ma=U/C$, represents the ratio between motion forces and fluid compressibility. A low Mach number, $\ll 1$, means a weak compressibility while an important Mach number signifies that compressible effects must be accounted for.

Those three numbers enable to make a clear distinction between the physic associated to the jet zone and the one of the whole ventilated infrastructure, without this jet. It appears through these dimensionless number that velocity effects governs a highly compressible flow for the jet zone but that turbulence is moderate considering that the Reynolds number is around the transition criteria. On the opposite, the flow in the ventilated infrastructure is characterized by an important turbulence level but a weakly compressible flow with a great influence of gravity. So, it appears that physical issues are different depending on the interest zone. Two next paragraphs discuss respectively on jet modelling regarding the physical characteristics and existing techniques and on flow modelling for the whole infrastructure.

2　Gases Jet Modelling

Several ways are available to model jet flows. Because a CFD approach is used for modelling dispersion in the whole domain, it is legitimate to wonder about its capability to be used from the release to the exhaust.

2.1　CFD Capability for Jet Modelling

If modelling high pressure jet for liquid or gas is a challenge for the CFD approach considering the complexity of the associated phenomena, some approaches were developed for particular configurations[8]. Because of the characteristic size of the injection jet, suitable mesh is required to model the different phenomena even if turbulence is quite low. Considering this characteristic size, in the

order of mm up to cm, this implies mesh to respect those characteristics with cell size in the order of mm or minus. On top of that, considering a 1mm cell with 300m/s velocity, it is possible to evaluate the order of the time step for such a modelling based on the CFL criteria. This CFL condition means a relation between velocity, spatial discretization and time step: $U\Delta t/\Delta x < 1$[9]. Consequently, for the above mentioned characteristics of the jet, the time step has to be in the order of 10^{-6} s. Furthermore, solving such a physic requires particular numerical techniques to be able to compute highly compressible flow. So, it appears that computing such thin important gradients requires a fine mesh. Because of the size of the domain to be model in the context of accidental gas dispersion, using such a mesh is not realistic and it is required to couple a jet flow model with the CFD simulation tool.

In the context of our study, that consists in modelling the jet inside a large infrastructure during quite long period that can reach one hour, this leads to unrealistic configuration. It then appears that the jet zone cannot be modelled, in the whole geometry, using a CFD approach. This implies introducing a coupling technique between two approaches. Consequently, a 1D jet model that enables to describe the leak behaviour from the hole to a low velocity zone is used to predict the jet evolution in the first centimetres.

2.2　2D Jet Model

Physic that occurs inside a high pressure release jet is highly complex and several studies were achieved to improve this phenomena description[10]. Mainly a complex sequence of shock waves can be produced. These shock waves will of course influence the flow and consequently the jet expansion. As shown in previous studies[11], a high pressure jet can be split into three zones: (1) A shock area with flow instabilities; (2) A transition zone; (3) A fully developed region.

This can be schemed, following[11] as reproduced on Fig.2 for weakly under relaxed jet with oblique shocks. In this case, the jet relaxed in the ambient to the atmospheric pressure through a series of shock waves.
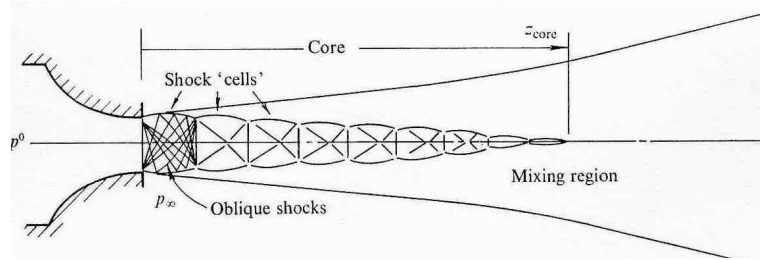

Fig.2　Schematic representation of the jet zone

Such a configuration is very complex to model and several works were achieved to obtain a description of the near filed, mainly[12][13] or, more recently[14]. It consists in computing a "pseudo-source" with an equivalent diameter that aims representing the jet flow after this complex wave's zone. The Birch's model was used to describe the first zone of the jet and computed equivalent diameter based on an isotropic approach, equation (1).

$$\frac{D_{eq}}{D} = \left(C_D \frac{P_{Res}}{P_0} \left[\frac{\gamma-1}{\gamma} \right]^{\frac{\gamma+1}{2(1-\lambda)}} \right)^{1/2} \left(\frac{T_0}{T_{res}} \right)^{1/2} \tag{1}$$

After having computed this equivalent diameter and characteristics at this diameter, a classic 2D analytical method for jet velocity and concentration evolution can be used. Some studies[10] have shown that velocity and concentration profiles can be approximate using Gaussian curves function of the centreline value. The centreline values are proportional to d_0/x. Then, a full set of equations is available to compute the 2D jet expansion, (2) and (3).

$$u_m(x)/U_0 = k_u(d_0/x) \tag{2}$$

$$c_m(x)/C_0 = k_c(d_0/x) \tag{3}$$

And then the Gaussian profiles are given by equation (4) and (5).

$$u(r)/u_m = \exp\left(-K_u \left(\frac{r}{x} \right)^2 \right) \tag{4}$$

$$c(r)/c_m = \exp\left(-K_c \left(\frac{r}{x} \right)^2 \right) \tag{5}$$

2.3 Identified limitation

This model of course induces some simplification in terms of solved physical phenomena. The jet evolution from the hole to the equivalent diameter can be assumed as well reproduced considering in this zone exchanges with ambient are weak. In the following mixing region, if the jet is well solved considering the air entrainment inside with the concentration and velocity distribution, the momentum transfer from the jet to the ambient is not modelled as the air well term due to jet entrainment. Of course this induces approximations about the velocity distribution close to the jet region. It must be however kept in mind that the objective of this work is not the jet prediction but the evaluation of the concentration distribution in large infrastructures. For this objective, it is considered as first approach that this momentum transfer can be neglected.

The second drawback of this model is that jet turbulence is not taken into account. Considering the characteristics of this zone, mainly the Reynolds number, it appears that turbulence of this zone is not as important as the one of the whole domain. This means that the turbulence source term form the jet to the domain can be neglected and consequently it is not modelled with this approach.

3 CFD Modelling of the Infrastructure

Computational Fluid dynamics (CFD) is a powerful tool to design safety measures but it must be kept in mind that such an approach still has some limits that must be known before achieving some modelling. The aim of this section is to provide a short overview of the CFD approach centred on the limits for gas dispersion modelling. The CFD general basis is the set of continuity equations: mass, momentum and energy. These equations cannot be solved explicitly, excepted for some ideal cases, and some sub models are required. The main one concerned the turbulence modelling. This model is detail in the first paragraph of this section because it impacts directly the dispersion modelling. Finally, the second paragraph of this section concerns the numerical solver. The one describes in this paper is the FDS one because of the available LES model of this code. The main interest of this numerical description is the underlining of the limits induced by this numerical approach.

3.1 Turbulence Modelling: LES Approach

These instantaneous equations require to be solved with a very fine mesh because their resolution implies to capture all the turbulent scale of the flow from the integral to the Kolmogorov one. Turbulent scales are going from integral scale to Kolmogorov one. Integral scale, l_t, is given by: $l_t = \dfrac{\nu . \mathrm{Re}_t}{u'}$ while the Kolmogorov one is: $\eta_k = \left(\dfrac{\nu^3}{\varepsilon}\right)^{1/4}$, corresponding to a unity Reynolds number. Of course, solving the whole turbulence spectrum is not realistic for industrial configuration. Modelling the whole scales requires the mesh to be fine enough to capture all those length, consequently, the number of cells requires in such a case is in the order of $\mathrm{Re}^{9/4}$[9]. For the present case, considering a 10^6 Reynolds number, this requires more than 3.10^{13} cells. It is then possible to deduce that, this commonly called DNS (Direct Numerical Simulation) approach, cannot be used for dispersion modelling. Some approximations have to be made. It also must be considered that large scales contain the major part of the turbulent energy, which means that they govern the flow. On the opposite, smaller scales are responsible of the turbulent energy dissipation. On top of that, if large scales are not isotropic, small scales becomes isotropic and consequently can be modelled.

Two approaches are available: the first consists in averaging the equation using a statistical tool (RANS: Reynolds Average Navier Stokes), the second consists in filtering equation to solve large scale and model the small ones (LES: Large Eddy Simulation). Because of the importance of the time dependence for such a phenomenon and the importance of large structure in the gaseous species transport, the LES approach was chosen.

The LES approach requires introducing a filter on the equation[1]. This filter consists in a cut off length in spatial space or in a cut off frequency in the energy diagram. Applying such a filter on the flow equation lets appear some cross correlation to be modelled while large scale quantity can be solved.

Solving the opened cross correlation means determining the turbulent energy transfers from large to small scale. Several approaches exist from static to dynamic ones. The objectives of this paper is not to detail the LES approach that can be find in [1] but to examine the limitation that can be generated by such an approach for dispersion modelling. For both modelling approach, the sub grid viscosity is written as a function of the Smagorinsky constant, C_s and the width of the filter

$$\nu_t = (C_s \varDelta)^2 \sqrt{2 \overline{S}_{ij} \overline{S}_{ij} - \frac{2}{3} (\nabla . \overline{u})^2} \tag{6}$$

The filter size is directly governed by the mesh but the Smagorinsky constant have then a real impact. Let first consider the static approach that is commonly used. In this case, the C_s value is fixed before the simulation. So, this means that the energy transfer from large to small scales must be evaluated a priori. If this value is well known for an homogeneous isotropic turbulence, the value for a complex industrial flow is highly difficult to predict. Furthermore, this value is flow dependant and consequently, its value will vary along time and space. This is the objective of dynamic model to compute its value. However, the complexity of those models is higher and such a model was not used in this paper. So, the limitation of the LES approach appears clearly and mainly concerns the choice in terms of C_s value. However, this description lets appear the mesh size importance considering that, if the cut off frequency is not in the inertial zone, the model is not consistent. Those two problems must be referred both for numerical model construction and results exploitation.

3.2   FDS Description: Numerical Method

The numerical description of above mentioned equation is one key parameter for CFD. Depending of the numerical scheme that is retained, some limitation should appear. The CFD tool that was used in the present study is the Fire Dynamic Simulator (FDS)[5][6]. This code is especially dedicated to fire modelling and consequently contains some hypothesis about the flow that enables to simplify the numerical approach. The main one is a low Mach number hypothesis that induces incompressible flow. This hypothesis enables to separate pressure in an average part and a fluctuating one. This numerical approach induces that high release velocity cannot be capture using the CFD code.

To complete the description, it must highlight that FDS is based on a first order finite difference spatial numerical scheme coupled with a two step predictor corrector temporal solver.

3.3   Synthesis of CFD Benefits and Limits

The brief CFD description given in this paragraph has highlighted several limits for accidental gas release in an enclosure. First of all, it was discussed the utility of the LES approach for turbulence modelling because of the importance in solving the unsteady phenomena with peak values instead of the average ones. However, using LES induces some constrains, mainly on the mesh that governs the filter size. This size must be in the inertial zone to have a correct numerical model. The second limit concern the Smagorinsky constant that is well known for a Homogeneous Isotropic Turbulence but a priori unknown for other flows. It must be considered however that, in the case of a large infrastructure, the turbulence can be assumed as quite isotropic and homogeneous and that the constant is around 0.2.

The last hypothesis is more specific to the CFD code used in this study, FDS and concerns the law Mach number hypothesis. This hypothesis is in accordance with the choice of using an algebraic model for the jet. The results of the jet model are used as boundary condition in the CFD code by creating a source with a dimension as computed by the model with given velocity and concentration distribution. As discussed previously, this approach does not make possible to account for momentum transfer along the jet zone, from the hole to the virtual source and for turbulence transfer from jet area to ambient.

4   Confined Dispersion: a Experimental Validation

The aim of this paper is to discuss about the LES capability for dispersion of toxic gases inside building equipped with a ventilation system. To validate this capability, CFD results is compared with experimental measurement obtained in an 80 m^3 room of INERIS.

4.1   Experiment Description

The INERIS 80m^3 room is a 5m long, 4m width and 4m height and is equipped with a ventilation system that enables to control the flow rate through the room. This room is schemed on Fig.3 where photography is also given.

This scheme shows the operational room located upstream the building. This operational room enable to install the measurement apparatus and all other control system. In order to homogenise ventilation inside the building, a wall is positioned near the entrance in order to prevent from a fresh air jet formation. This aims to have a well distributed flow inside the building.

Fig.4(b) presents the sensors distribution inside the room. Six vertical measurement lines are distributed inside the building, each line is equipped with three gas detectors and 5 thermocouples located at different height, Fig.4(a).

A large series of experiment were achieved but, for the present source model, only gas release can be modelled. The above described jet model is not yet able to deal with two phase flow and consequently, only two experimental configurations can be modelled. These two configurations correspond to different releases and different ventilation regimes. The first configuration is a 4.4g/s gaseous ammoniac release with a 2000m³/h ventilation rate. For the second configuration, the ventilation flow is only 500m³/h for a 2.2g/s ammoniac release. So, ventilation flow rate fore the second case is divided by 4 while the ammonia injection rate is only divided by 2. This release is achieved in both cases through a 2mm hole.
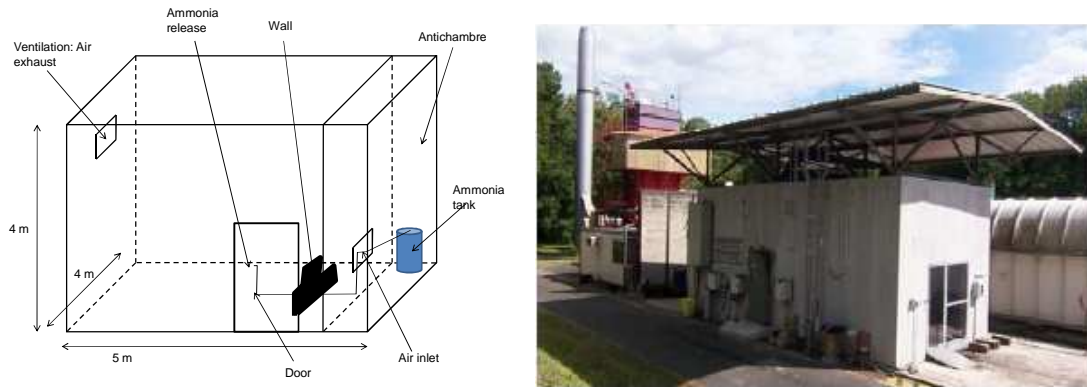

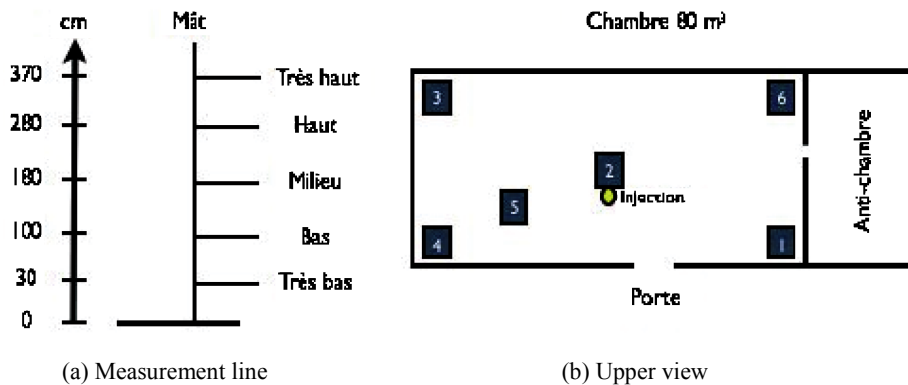**Fig.3   Scheme and photography of the INERIS 80 m³ room**

(a) Measurement line   (b) Upper view

Fig.4   Sensors distribution in the building

4.2   Numerical Model

As discussed in the first part of this paper, an important point for an LES modelling consists in defining the cell size in the turbulent inertial zone. This implies defining the turbulent scale representative of the flow. Doing this, the starting point is the Reynolds number. For this flow, the Reynolds number is of about 100000, this means that the Kolmogorov scale, proportional with $(1/Re)^{3/4}$, is in the order of $1.6*10^{-4}$ m. The Integral scale is in the order of half the room width, i.e. 2m, that represents the larger scale than can be encountered in the domain. It must be important to keep in mind that the objective is not in reproducing the jet dynamics but the ammonia dispersion inside the room. Considering that 1/20 of the integral scale is in the inertial zone, this implies cells to be lower than 0.1 m. This value was used to define the mesh with 0,1 m cells. This size enables to filter the fluid equations in the inertial zone and consequently respects the LES requirements with 120000 cells.

The second point to be checked in the numerical model is the Smagorinsky constant. Considering that, because of the ventilation coupled with the injection, turbulence is 3D, the 0,2 standard value was kept. This will be discussed according the results. The results for the two ventilation configurations are described next.

4.3   Comparison Between Experimental and Numerical Results: 4,4g/s Release

As mentioned above, the fist experiment that was modelled corresponds to a 4,4 g/s release with a ventilation flow rate of

2 000 m³/h. Fig.5 shows the ammonia distribution inside the room 240 s after the release start. This figure is interesting because it shows the position of the virtual source and the dynamic of the ammonia jet that impinging the wall. As shown on this picture, the virtual release is quite far from the real source and consequently bigger than the real hole. However, according the jet sub model, the characteristics of the jet is maintained and enables to achieve a realistic computation.

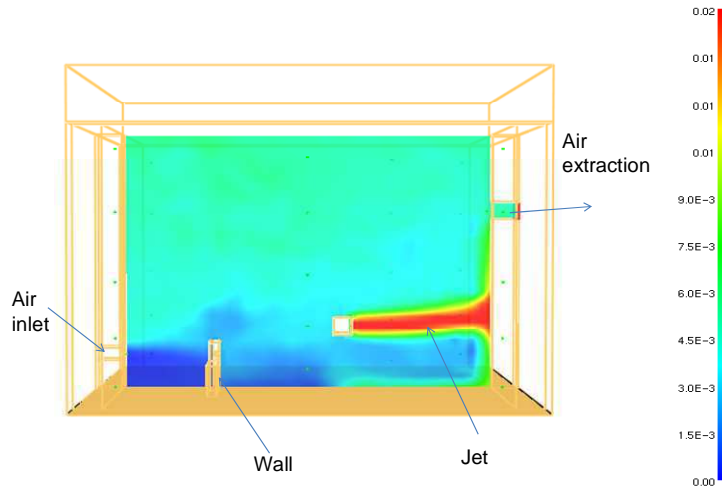Concentration at the top and at the bottom of positions 1, 3, 4 and 6 are presented on Figs. 6 and 7.
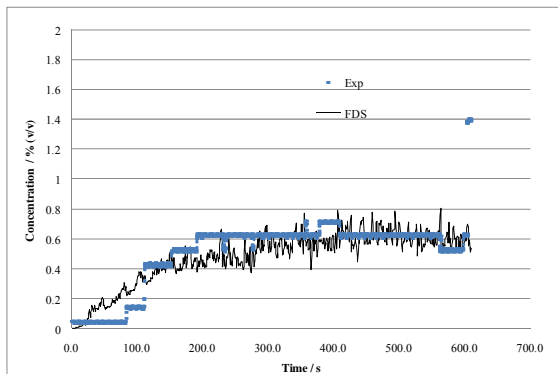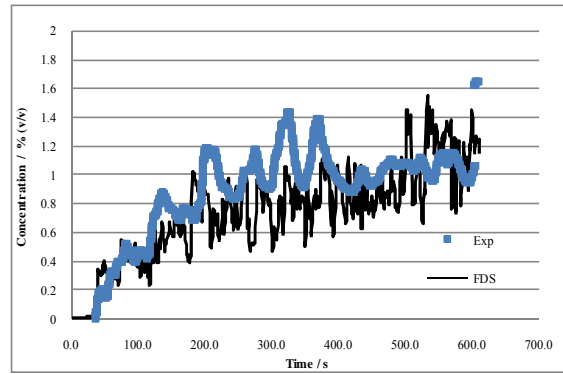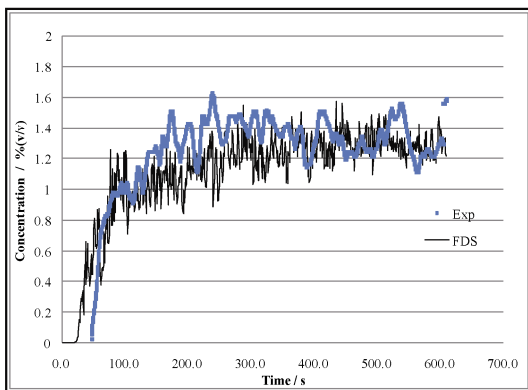

Fig.5   Visualization of the results: ammonia mass concentration 240 s after the release start

(a) Position 1

(b) Position 3

(c) Position 4

(d) Position 6

Expe: points; Simulation: line

Fig.6   Evolution of ammonia concentration versus time for upper of position 1, 3, 4 and 6
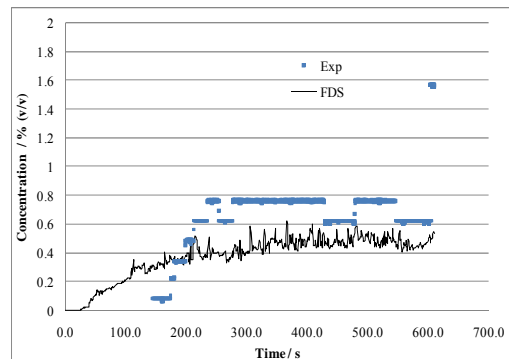
(a) Position 1

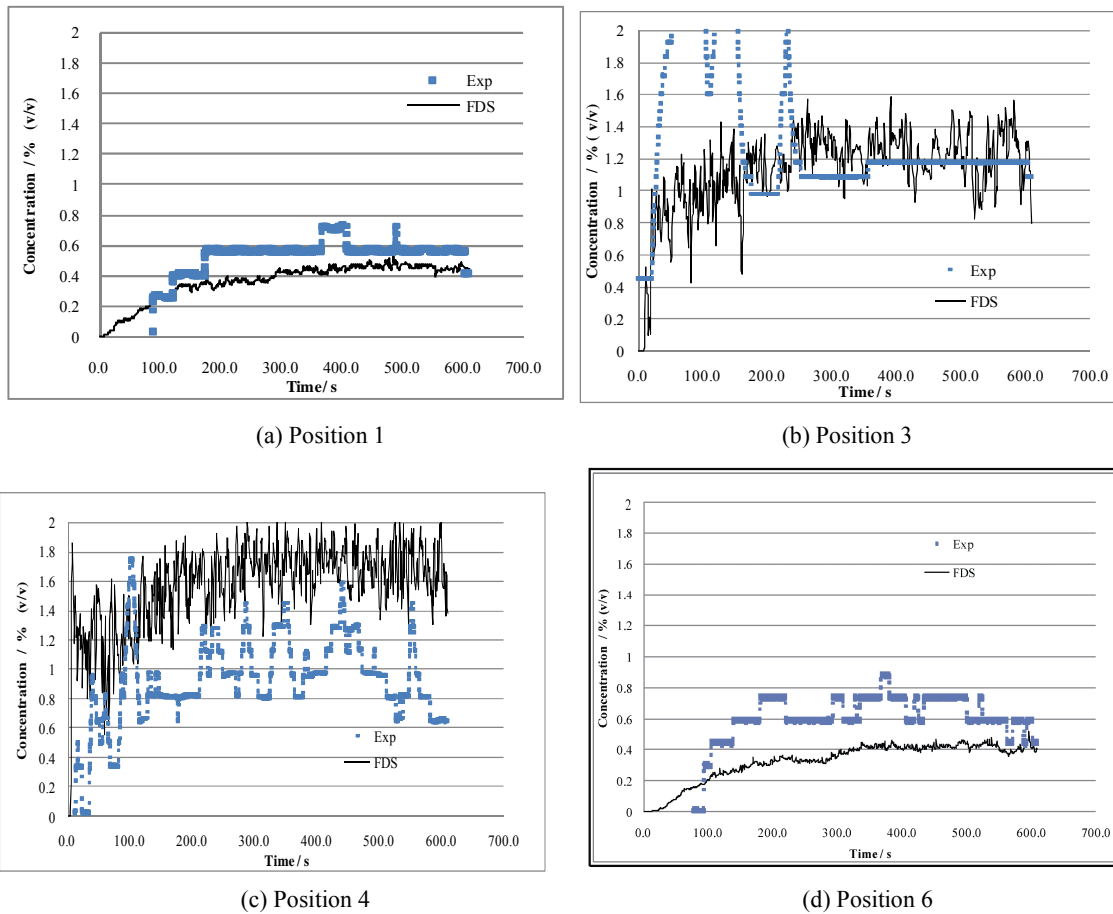(b) Position 3

(c) Position 4

(d) Position 6

Expe: points; Simulation: line

Fig.7   Evolution of ammonia concentration versus time for lower of position 1, 3, 4 and 6 (bottom right)

First, the results for the upper part of the measurements sections, is in great agreement with the experimental results even with the hypothesis described at the beginning of this paper. The second series of results, the lower point of each corner measurement position, shows a quite good agreement but with one main difference. It is also important to keep in mind that the experimental incertitude is around 30%. The main difference concerns the 250 first seconds of the upper values on the upper point of position n°3. This part corresponds to a quick increase of the concentration in this domain that can be due to the dynamic of the jet. This dynamic cannot be reproduced by the CFD code and consequently, this first phase is not well reproduced. The important increase is however quite surprising because this is the only one sensor that shows this increase. On top of that, the concentration after those 250 s is quick well reproduced.

Finally, considering the importance of a ventilation system in such an equipment and the impact that a gas can have on this system, the prediction of the concentration at the entrance of the ventilation system was compared with the experimental value. According this first series of comparison that seems encouraging, it is interesting to go any further with the second configuration experimental and numerical comparison (Fig.8).

This curve shows that the value at the entrance of the ventilation system is quite correctly predicted using the simulation code FDS. The difference observed in the 250 first seconds can be explained by the sensor dynamic and the discrete measurement. Once again, it is important to note that the sensor error is around 30%.

4.4   Comparison Between Experimental and Numerical Results: 2.2 g/s release

The difference between the previous case and the present one is the ventilation flow rate and the injection rate. The injection is, for this case, 2.2 g/s while the ventilation flow rate is diminished to 500 m3/h. The dynamic of the flow is quite not modified and, mainly, the integral scale can be still estimated to the half size of the room. As for the previous case, the evolution of concentration for the upper and lower sensor for each corner of the room is plotted again the predicted value, Figs. 9 and 10.

This second series of comparison curve show again a god agreement between experimental results and numerical ones. Only the prediction of concentration on the lower sensor of position 4 is far from measurements. It is important to note that, on this curve, the first part of the experimental curve is not plotted because values are negative, around -0.2. This may indicated either a sensor default or a concentration out of the range. Conclusion is the same and this point cannot be exploited placidly. This second series of comparison shows a great agreement between experimental values and numerical predictions. The simulation FDS code is able, not only to predict the steady values but the unsteady evolution to.
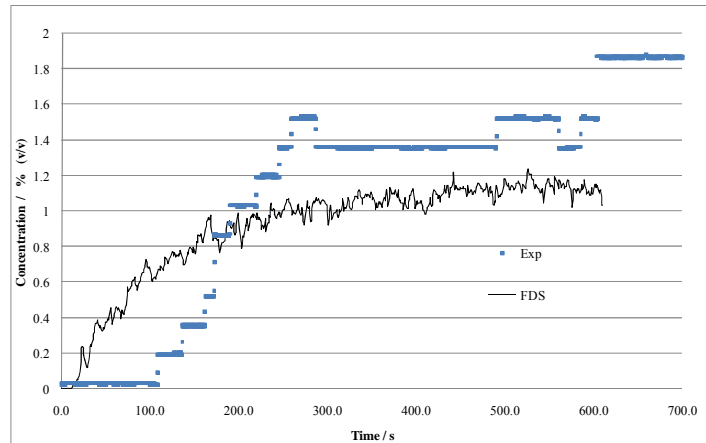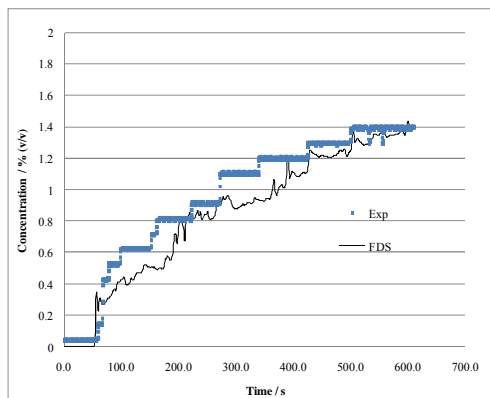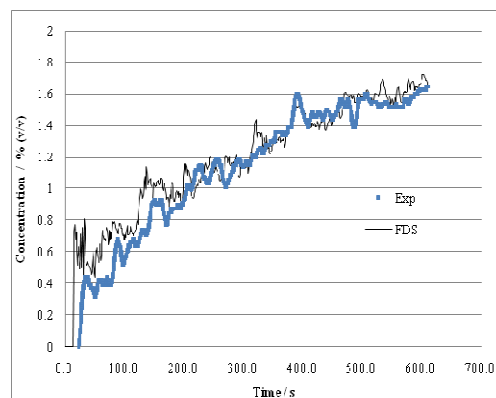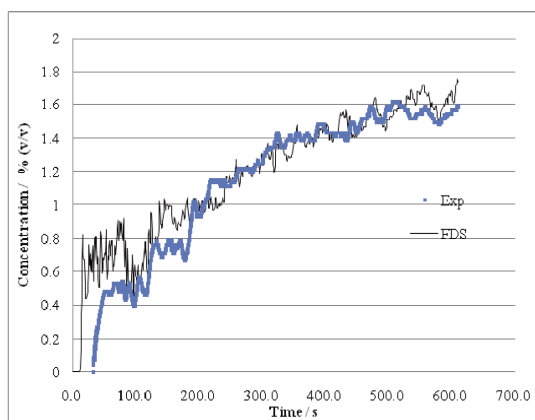

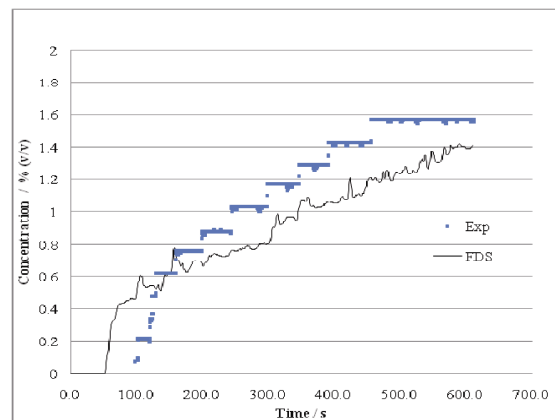**Fig.8   Evolution of the concentration at the entrance of the ventilation system**

(a) Position 1

(b) Position 3

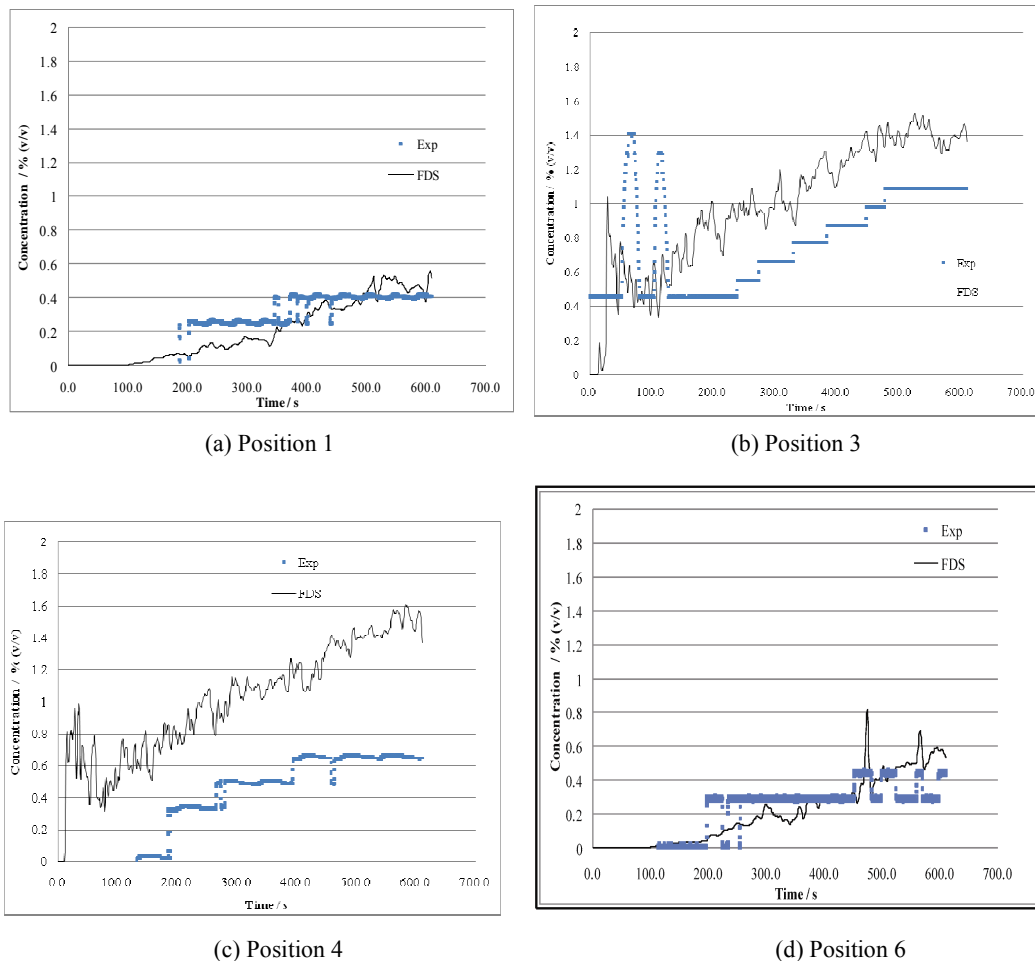(c) Position 4

(d) Position 6

Expe: points;   Simulation: line

Fig.9   Evolution of ammonia concentration versus time for upper of position 1, 3, 4and 6

4.5 Evaluation of CFD Capability: Synthesis

In the introduction of this paper, two main criteria were identified as critical for CFD modelling. First and second concern the turbulence modelling: filter size and Smagorinsky constant. Finally, the jet model influence must be discussed.

To evaluate the first, a simulation was achieved with a finer mesh, 420 000 cells and a highly finer mesh, with 2 250 000. Those two simulations have shown a weak influence of this parameter on the predicted concentration. However, the finest mesh has shown the LES ability in capturing small turbulent scale. Consequently, the concentration evolution curve is noisy; this can be explained by the fact that smaller cell size implies smaller scale to be captured with a smaller characteristic time. Such high frequency cannot be captured by gas sensor that gives an averaged value.

The second parameter is the Smagorinsky constant that was kept to the 0.2 standard value considering a 3D flow, and consequently, a 3D turbulence decrease. Because the lack of data concerning velocity fluctuation, it is not possible to construct the experimental turbulence spectra that can confirm this value. The concentration comparison on the different position confirms that the flow is correctly reproduced because values are correct in the four corners of the room both in the upper part and in the lower part of the room. Consequently, for the present dispersion case, this choice appears to be valid. Simulations achieved with lower values have shown that this has, as assumed, a weak influence on the result, which signified that resolved scales are responsible of the mixing. Finally, as discussed above, the jet sub model induces a momentum loss because one part of the kinetic energy to be transfer to the ambient air before the virtual release. It appears that, this part of the momentum is not crucial for gas dispersion prediction in a ventilated enclosure.

(a) Position 1	(b) Position 3

(c) Position 4	(d) Position 6

Expe: points; Simulation: line

Fig.10   Evolution of ammonia concentration versus time for lower of position 1, 3, 4 and 6

Finally, it appears that, even if some approximation are made for computing high pressure gas release in an enclosure, FDS is quite correctly able to predict concentration distribution inside the whole room.

5 Conclusions

This paper describes a methodology to model gaseous release in large infrastructure, from the source to the whole domain. Because of the complexity and characteristics of jet near the release, CFD cannot be applied to the whole domain. An algebraic model form the literature is used before introducing the results in the FDS CFD code to model the dispersion inside the infrastructure. The jet model enable to predict the concentration and velocity in accordance with the CFD model limits while keeping the major information: velocity and concentration. After introducing this in the CFD code, turbulence phenomena in the domain is model using a LES approach to capture the large scale effect and obtain the unsteady characteristics of the flow.

This coupled methodology was compared with experimental data for two cases of ammonia release in a ventilated 80 m³ room. Sensors were distributed inside the room to follow the concentration evolution along time. The comparisons have shown that, for both case, a great agreement between experimental measurements and numerical prediction. This signifies that, while some phenomena are not accounted for, the global behaviour of the gas dispersion inside the domain is correctly predicted. These comparisons have also shown that, even the uncertainties on several parameters as Smagorinsky constant, the flow is sufficiently well reproduced to have a correct prediction of the concentration field in the domain.

Finally, the proposed approach seems valid for such an application and can be extended to real configurations for both accidental hazards and intentional threats.

Several perspectives are identified for future work to improve this approach. The first concerns the jet part for which turbulence, momentum and air transfer with the ambient can be introduced in order to evaluate the influence. Concerning turbulence, because LES is used, turbulence is not just boundary conditions on certain quantities as for RANS approaches but it consists in the time fluctuation of the different physical values. Doing this requires to be able to determine the characteristic frequencies of the flow, through for example a Strouhal number. For the momentum and air transfer, it consists in a boundary condition on the mass and momentum equation through a well term of air function of the entrainment characteristic of the jet and a shear velocity determined using the algebraic law.

Then, because not only gaseous toxic can be release, a two phase sub model must be evaluated. However, in this case, the momentum quantity transfer to the gas will probably not be neglected and such an improvement will come later.

The second perspective aims in improving the CFD modelling and mainly turbulence. This can be done, for example with the dynamic LES model that enable to compute the energy transfer from large to small scale as a function of the flow. Such an approach is more realistic than a constant in the whole domain.

Finally, if this approach was developed for confined dispersion, it is also suitable for atmospheric dispersion. In such a configuration, the domain characteristic dimensions are not on the order of hundred meters but in the order of kilometres. The problematic is next quite similar considering the main part of the turbulent energy is the atmospheric turbulence that governs the gas dispersion. However, some other problems have to be solved before achieving such a computation: atmospheric turbulence description, influence of the roughness and the LES wall law problematic.

Notations

Symbol	Meaning	Symbol	Meaning
[C]	Gas concentration	r	Radius
c	Sound speed	T_0	Ambient temperature
C_0	Origin concentration	T_{res}	Tank temperature
C_D	Discharge coefficient	U	Velocity
CFL	Courant Friedrich Lewis number	U_0	Origin velocity
C_s	Smagorinsky constant	u'	Velocity fluctuation
c_m	Centreline concentration	u_m	Centreline velocity
D	Hole diameter	x	Centreline position
D_{eq}	Equivalent diameter		
Fr	Froude number		Isentropic coefficient
g	Gravity force		filter size
L	Length	k	Turbulent Kolmogorov scale

Symbol	Meaning	Symbol	Meaning
l_t	Turbulent integral scale		Dynamic viscosity
Ma	Mach number		Kinematic viscosity
P_0	Ambient pressure		Density
P_{res}	Tank pressure	t	Time step
Re	Reynolds number	x	Cell size
S_{ij}	Resolved strain rate tensor		

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