HARMONIZATION OF PRACTICES FOR ATMOSPHERIC DISPERSION MODELLING WITHIN THE FRAMEWORK OF RISK ASSESSMENT

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Abstract:
Since many years, using tridimensional (3D) models is increasing in order to compute hazardous consequences of dangerous phenomena such as fire, explosion or atmospheric gas dispersion and then estimate safety distances. In the specific context of the French regulation and mainly for the land use planning in the neighbourhood of industrial facilities as depicted in the Technological risk prevention plan (PPRT), prediction of safety distances is a key issue. First computations that were achieved has highlighted discrepancies between atmospheric 3D models (CFD, mass consistent, ...) results but also with conventional approach as Gaussian or integral models. In order to prevent such discrepancies and to enlighten scientific reasons of those differences, a French working group was created in November 2009 on the demand of French Ministry of Ecology and Sustainable Development. To reach these objectives, several simulation benchmark tests were carried out. In a first part we present the benchmark tests as well as their interpretations and we describe efforts of harmonization on practice and input data. In a second part we focus on the scientific analysis to perform more homogeneous input data between the several kinds of 3D atmospheric dispersion models. Some of the best practices and requirements are presented and discussed in the last part.

Key words: *safety distances regulatory studies, CFD, mass consistent, Gaussian model, integral model, blind tests, tridimensional (3D) models, harmonization.*

INTRODUCTION

Context: Industrial risk management in France

On September 21, 2001, a huge explosion occurred in Toulouse (at the AZF factory) causing 31 deaths and thousands (~ 2500) of injured people. Two years after this major industrial accident, a new law was introduced on July 30, 2003 which described both prevention and repair of the damage caused by industrial and natural disasters. This law was the starting point of a general regulatory environment, then regulations have been made considerably tighter and the entire approach towards risk assessment has changed (Lenoble and Durand, 2011). The Technological Risk Prevention plan (PPRT in French, standing for Plan de Prévention des Risques Technologiques) is the new legislation tool aiming to protect people by acting on the existing urbanization and also by controlling the future land-use planning in the vicinity of the existing Seveso establishments. The identification of potential scenarios is the first step of the numerous one required along the process of the PPRT elaboration. For a physically possible scenario, this analysis is then followed by the prediction of potential consequences (dangerous phenomena). The prediction of the impact area (thermal, overpressure and toxic effects), which is generated by a dangerous phenomenon, is another required stages. The prediction of effects distances is always performed using computational tools. Atmospheric dispersion models are then required to predict distances or impacted zones by toxic or flammable products. When the PPRT is finalized, it delineates a risk exposure perimeter, at the heart of which regulated zones are established. Among these zones, areas can be defined for expropriation or for protective measures on buildings which can be compulsory. Due to the new legislation the stakes are higher and this highlights the importance in computing precise distances to prevent from people exposure while assessing realistic safety cost. Predicting models used in this framework are characterized by a large variety of nature and complexity. For the same analysed hazardous phenomena considered, discrepancies appeared in terms of computed distances or impacted zones between atmospheric 3D models (CFD, mass consistent, ...; *tridimensional model* means other than integral or Gaussian models) results but also with conventional approaches as Gaussian or integral models. What are the parameters that can explain these discrepancies between those computations? Actually, reasons are numerous and of different types. The reasons generally put forward are given in the list below, however this list is not exhaustive:

1. Differences between hypothesis and difficulties to be implemented as input data for dispersion models,
2. Emission term source is estimated following distinct approaches,
3. Intrinsic feature of dispersion atmospheric model : gaussian, integral, CFD, mass consistent, lagrangian,
4. Regardless input data, implementation of atmospheric dispersion models of same feature may strongly differ,
5. Results can be identical but interpretations in terms of effects distances are not equivalent.

Items 1, 3 and 4 are particularly quoted when 3D atmospheric dispersion models are used. Indeed, since many years, the use of 3D models is increasing in order to compute hazardous consequences of toxic/flammable gas dispersion. Particularly, one often argue that this kind of models allow to take into account complex environment (presence of obstacles) on the process of atmospheric dispersion in contrast with the traditional models. In order to prevent discrepancies between atmospheric dispersion modelling and to enlighten scientific reasons of these differences, a French working group was created in November 2009 on the demand of French Ministry of Ecology and Sustainable Development.

Objectives of the French tridimensional atmospheric dispersion working group

The objectives of this group were to explain scientific basis of 3D atmospheric dispersion modelling in order to justify links between results and input data or sensitive parameters, to create a guideline of best practices for 3D atmospheric dispersion modelling with the objective of forecasting hazardous consequences within the framework of risk assessment and to provide a reading tool for the administration in charge of the evaluation of the above mentioned studies.

METHODOLOGY AND PURPOSE OF TEST CASES

A 3D computation requires to carry out five main stages that are illustrated in Figure 1.

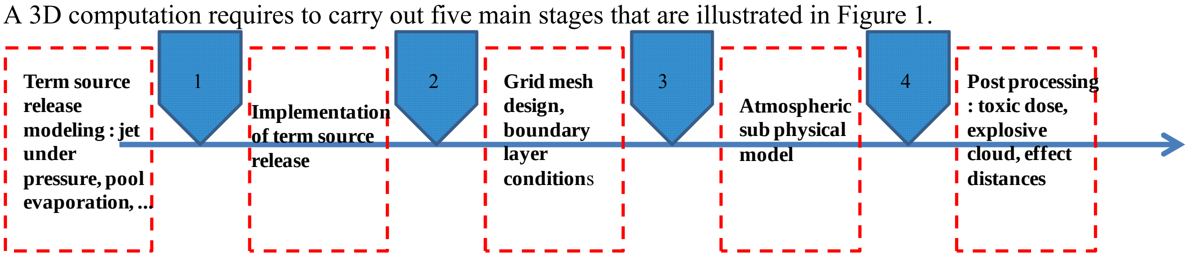

Figure 1 : Main calculation stages to simulate atmospheric dispersion of an accidental release (toxic or flammable gas release)

In order to assess the influence of the whole set of calculation stages on final results, three tests cases, including two fully blind tests, were achieved by working group partners with their own model. Significant stages were identified: implementation of source term emission, choice of calculation domain, mesh generation, boundary conditions, choice of physical sub model. The term source release modelling is one of the most important steps in such an approach but not only for 3D modelling. However source term modelling was not considered within the scope of the study which focused on atmospheric dispersion modelling. The test cases computed by the different participants were used to elaborate good practices. About 12 modellers have participated to this exercise by using mainly k-ε based model. On top of that, other RANS and LES approaches and mass consistent models were also used. For each test, efforts of harmonization on practice and input data were performed. Those computations were used to highlight the main reasons of discrepancies and to elaborate new requirements

Sum up of test cases

As a first blind test, a fictive gas release in a free field was chosen. Three gases were studied: heavy, neutral and light gases. The set up of the release is expected to characterize a line rupture (2 inches diameter) on a vessel under pressure (8 bars). A ten minutes release was computed in the wind direction. Following French regulatory requirement (Circular of May 10, 2010) two meteorological conditions, which are characterized by Pasquill classification and wind module (F3 and D5), were modelled. As in regulatory studies, the definition of the first test case was limited to source term definition, atmospheric stability and wind definition. Modellers were free to set up others calculation parameters needed for the simulation. This first test case results clearly showed great discrepancies in the results, focused on toxic effects distances, because the way of using the 3D models was specific to each user. Some results are presented in Figure 2 and illustrate that for a low evolution close the toxic threshold a weak difference between calculations can lead to a substantial difference in terms of distance.

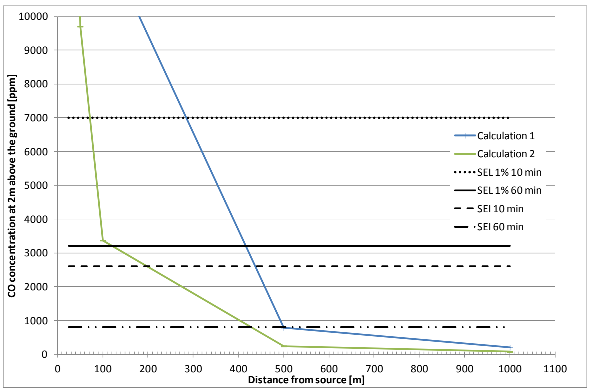

Figure 2 : calculated concentration of CO at 50 m, 100 m, 500 m for two calculations of the first test case ; SEI 10 min stands for *Seuil effet irreversible* is the threshold of irreversible effects for 10 min exposure; SEL 1% stands for *Seuil effet létal* is the threshold of first lethal effects above which 1% mortality can be observed in the exposed population

This aspect is the basis of the hereafter discussion. It confirms a need to standardize the methodology, four major factors were identified: interpretation of input wind profile for 3D, turbulence models, mesh and cells size, source term implementation. The following blind test was performed in order to investigate the influence of these factors to prediction calculations. This second fictive test case consisted in modelling a massive release of propane (emission rate of 45 kg/s) in an obstructed field. This massive release is supposed to produce an unconfined vapour cloud explosion. A series of obstacles were introduced inside the domain. First, two factors were fixed: inflow wind, temperature and turbulence profiles, then, the source term was simplified. On top of global results comparisons, specific comparisons were made to evaluate the impact of some identified specific factor. Then, two main turbulence modelling approaches were evaluated: RANS and LES. In using similar code, differences on results were observed due to factors: buoyancy effects taken into account or not in the turbulence modelling, obstacles roughness modelling, surface or volume source term implementation, and the mesh. Although discrepancies were observed in terms of gas volume and explosive mass it is important to keep in mind that the final results associated to the explosive gas release, i.e. overpressure distances, are less sensitive to the dispersion modelling than prediction of toxic distances. Indeed, in some cases uncertainties on flammable cloud prediction calculations may sometimes be reduced by approaches used downstream to predict overpressure distances. This can be illustrated through the common approach, which is called Multi-Energy, to estimate overpressure distances that is based on a function of $M^{\wedge 1/3}$, with M the total mass of explosive gas.

Specific works were performed during this second fictive test to investigate the consideration of turbulence production by buoyancy effects and distance upstream the first obstacles. Based on those two first blind cases, the working group observed that progress had been made by the different participants by using common practices. After having defined most of those good practices, a third case based on an experimental case (Kit Fox field campaign) has been carried out to evaluate it. A concise list of good practices is given in a later chapter.

STANDARDIZATION OF INPUT METEOROLOGICAL PROFILE: RELATION BETWEEN PASQUILL CLASSIFICATION PROFILE AND CFD APPROACH

As mentioned previously, for atmospheric dispersion modelling in case of ground level release, French regulation requires a minimal set of atmospheric conditions defined with the traditional Pasquill scheme: F3 and D5. A roughness length is also required to characterize the environment of the industrial plants. It is obvious that such conditions cannot be translated easily to a 3D model approach. Having in mind that inlet profile is one of the key parameter, it was then decided to set up some rules in order to achieve the homogenization of the inflow boundary conditions. The relation between Pasquill classes and tridimensional inflow boundary conditions is difficult to establish because the classes of Pasquill represent a broad variety of possible states of the atmosphere, as illustrated by the well known diagram of Golder (1972) in Figure 3.

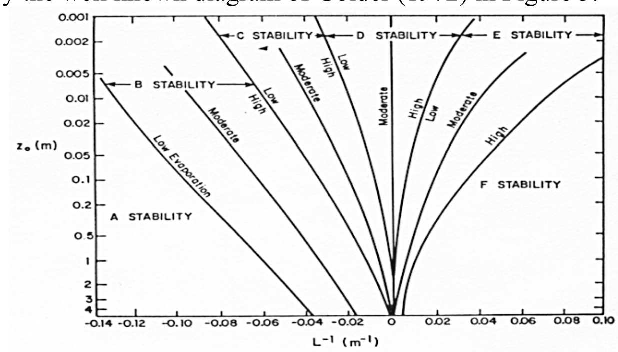

Figure 3: Relations between Pasquill stability categories and Monin-Obukhov length and surface roughness (from Golder, 1972)

For an atmospheric condition defined only with three parameters (Pasquill class, velocity module at reference height, and ground roughness) several profiles are then possible. It is clear that, whether integral and Gaussian models are commonly using highly simplified velocity profiles, 3D models need more sophisticated profiles for different physical quantities as wind, temperature and turbulence profiles. It is also obvious that, in most of the industrial cases, not only the surface boundary layer must be modelled but the entire atmospheric boundary layer one. For regulatory reasons and consistence with existing computation, it is important to limit the set of input parameters meteorological data as much as possible. Great work was performed by the working group to establish a consensus between current theories (Dyer, 1974; Panofsky and Dutton, 1984; Zilitinkevich, 2005; Gryning et al., 2007). In previous guidelines intended for environment around buildings (Tominaga et al., 2008), formulations were suggested to express profiles in the surface boundary layer where the assumption of constant shear stresses is valid. From similarity theory, under horizontally homogeneous and steady state conditions the wind profile follows the logarithmic law (Panofsky and Dutton, 1984, p. 134):

$$u(z) = \frac{u_{*0}}{\kappa}\left(\ln\frac{z}{z_0} - \Psi_M\left(\frac{z}{L}\right)\right) \tag{1}$$

Here κ (0.4) is von Karman constant, z is height above the ground, u_{*0} is friction velocity friction, u is mean wind speed, Ψ_M are the universal function of the stability parameter z/L, where L is defined as the Monin Obhukov length. While it gives a valid description of the surface boundary layer, this formulation is rigorously not valid above the surface boundary layer. In the scientific literature there are fewer proposals to extended profiles above this latter. As indicated previously, the working group has to pay a specific attention to these extensions in order to simulate a more realistic boundary layer flow. The approach proposed by the working group is based on the Gryning theory (Gryning et al., 2007) and could be described as follow:

1. First, following former approaches used for integral and Gaussian models, only 4 parameters are required: Pasquill Class, Wind module (u_{ref}) at height reference (z_{ref}), length roughness (z_0), ground temperature (T_0);
2. Next, the Golder approach allows to determine a value of Monin-Obukhov length. To establish a unique value of Monin-Obukhov length, it was decided to rely on formulation that express midpoint of Pasquill class:

$$\frac{1}{L}=\frac{1}{L_S}\log_{10}\left(\frac{z_0}{z_s}\right)$$

where for range $0.001 \le z_0 \le .0.5$, parameters Ls(m) et zs(m) are constants.

3. Finally, the Gryning approach is used to express wind profile within the surface boundary layer profile and above surface layer.

This leads to an iterative calculation to estimate the friction velocity near the ground, u_{*0} that matches with required wind module at height reference; kinetic turbulent energy and dissipation profiles are based on the equilibrium hypothesis. In the surface layer, the friction velocity u_{*0}, is considered constant as previous authors theory (Businger et al. 1971; Dyer 1974). Above the surface layer the local friction velocity has been considered to diminish with height, the following expression is used:

$$u_*(z)=u_{*0}\left(1-\frac{z}{z_i}\right) \tag{3}$$

with z_i the height of the atmospheric boundary layer. In order to keep a minimal of turbulent energy close to the top of boundary layer it was decided to consider a minimal value for $u_*(z)$ equal to 10% of ground local friction velocity. The wind profile is expressed following the most general formulation of Gryning's approach:

$$u(z)=\frac{u_{*0}}{\kappa}\left(\ln\left(\frac{z}{z_0}\right)+\frac{bz}{L}\left(1-\frac{z}{2z_i}\right)+\frac{z}{L_{MBL}}-\frac{z}{z_i}\left(\frac{z}{2L_{MBL}}\right)\right) \tag{4}$$

with L_{MBL} that express length scale in the middle of the boundary layer and z_i the top boundary layer. For stable conditions the most general formulation of L_{MBL}, can be expressed following formulation:

$$\frac{z_i}{L_{MBL}}=2\left[\left[\left(\ln\left(\frac{u_{*0}}{fz_0}\right)-B\left(\frac{u_{*0}}{fL}\right)\right)^2+A^2\left(\frac{u_{*0}}{fL}\right)\right]^{1/2}-\ln\left(\frac{z_i}{z_0}\right)-b\left(\frac{z_i}{2L}\right)\right] \tag{5}$$

with f the Coriolis parameter (f=1.10^{-4} s^{-1}). Gryning pointed out that these coefficient values are rather well established for the neutral atmosphere but their stability dependence is still matter of discussion (Zilitinkevich, 2005). Coefficient values of A = 10 and B = - 10 were taken from Tennekes (1973) by and correspond to stable cases. The working group concentrated its effort on this kind of conditions because they are conservative for a majority of regulatory studies but the whole approach can be adjusted to others conditions (neutral, instable). Above the top layer the wind velocity is fixed to value obtained at z= z_i. This latter is estimated by an analytical formulation (Garratt, 1992):

$$z_i=0.4\sqrt{\frac{u_{*0}L}{f}} \tag{6}$$

To evaluate the turbulent kinetic profile, the similarity functions proposed by Dyer (1974) for stable conditions were considered, the profile is specified as follows:

$$k(z)=\frac{u_*(z)}{\sqrt{C_\mu}}\sqrt{\frac{1+4z/L}{1+5z/L}} \tag{7}$$

The dissipation rate profile is based on hypothesis that viscous dissipation balances shear production and buoyancy. Hypothesis of local friction velocity was considered consistently with wind profile formulation.

$$\varepsilon(z)=\frac{u_*(z)^3}{\kappa}\left(\frac{1}{z}+\frac{4}{L}\right) \tag{8}$$

The turbulent viscosity, K_m, is expressed by:

$$K_m(z) = C_\mu \frac{k(z)^2}{\varepsilon(z)} \quad (9)$$

with C_μ the coefficient use to define the eddy viscosity in the k-ε model. Standard value for $C_\mu = 0.09$ and value recommended by Dyunkerke (Duynkerke, 1988) were tested by modellers. An application of this approach is being tested thanks the third test case performed by working group by comparisons with an experimental case. The Kit Fox field campaign, trial 5-8, that corresponds to stable conditions was chosen. As explained previously a set of minimum data was used: $u_{ref} = 4.1$ m/s, $z_{ref} = 4{,}88$ m, $z_o = 0.2$ mm, $T_0 = 301.8$ K, L = 8 m.

DISCUSSION ON BEST PRACTICES AND REQUIREMENTS

A list of numerous best practices, requirements on 3D dispersion model capabilities and users' skill to demonstrate it has been listed by the French working group. Some practices come from its own work: construction of the inlet velocity profile, definition of a validation procedure, range values of Schmidt coefficient and justification,...; others were already identified in previous guidelines (Franke et al., 2007) as the minimum distance between obstacles and domain boundaries, etc.

CONCLUSION

In this paper we presented the harmonization of practices for atmospheric dispersion modelling within the framework of risk assessment. The different classes of stability, required by the regulation, have to be constructed on the basis of equations established by the working group. If we focus on suitability of 3D models to simulate atmospheric turbulence in order to be in accordance with regulation, the demonstration of model capability to maintain wind and turbulence profiles through the free field calculation domain, up 2 km limit, is one of the main requirements. Knowing the complexity for CFD model to fulfil this requirement in a strictly way, it was decided that outlet profiles must show the same Pasquill class as input profiles. To conclude, it is worth noting that for some chemical products many uncertainties still exist in terms of acute toxic threshold values and scientific researches are going on this topic, which 3D models could allow foreseeing improvements by taking into account the intermittency of toxic cloud.

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