

Relevance of the current modelling methods for the prediction of LNG vapour dispersion and development to be carried on

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This paper shows comparisons between several commonly used software for gas dispersion modelling FLACS, CFX, PHAST and the experimental data collected during the large-scale dispersion tests of LNG vapour carried out at Montoir in 2013 by the ENGIE Lab CRIGEN. This paper aims to give guidelines for using FLACS and CFX codes for LNG vapour dispersion.

Background and Objective

ENGIE, leader in Liquefied Natural Gas (LNG) market, faces new safety challenges related to LNG process, transport and use.

In the framework of liquefaction processes, LNG storage and transport, or LNG use as a fuel, any accidental leak may lead to critical events ranging from cryogenic impact on personal and structures to flammable events such as fires and explosions. In this context, being able to predict LNG vapour dispersion is a key asset to evaluate potential flash fires which are the dimensioning hazard for the sitting and risk assessment studies.

Today, the main difficulty in assessing LNG vapour dispersion comes from the strong differences of temperature and density between the released material and the surrounding environment. Unlike the common belief that the LNG related hazards can directly be assimilated to ones studied in the past for heavy fuels such as gasoil, kerosene or LPG, the association of the extremely cold storage conditions, the low vaporization temperature and the light gas composition complicates the behaviour of the released material.

Today, in order to predict gas dispersion and adapt the design of the considered infrastructure, engineering companies usually use numerical or analytical models. These models are Computational Fluid Dynamics software (CFD) or simpler software like PHAST (DNV-GL). However, there has not been any real scale experimental campaign to validate these models for cold gas dispersion.

As a consequence, CRIGEN (ENGIE Research and Technologies Division) carried out in 2013 medium-scale experiments of LNG vapour venting to atmosphere, thanks to funding of ENGIE’s LNG BU and TOTAL (Sail, et al., 2015). Several vent pipes with vertical and horizontal directions and 6’’ or 18’’ diameters were used to release cold LNG vapour at around 5 meters high, with release rates between 1000 and 6000 kg/h. The objective of these tests was to gather experimental data on the shape and dimensions of LNG vapour plume (92-97% of methane), generated by venting : path of gas plume, temperature, dispersion and dilution, thanks to concentration measurements in CH4 and O2, temperature measurements and standard and infrared cameras.

Based on this experimental database, this article aims to show the abilities and the limits of different modelling tools and to highlight the further development to be conducted to complete and improve the accuracy of predictions. CFD has already shown its ability to improve the level of accuracy for heavy gas cloud dispersion with regard to standard integral methods, especially in order to be able to correctly consider the facility configuration and ground topology. However, the relatively recent use of CFD for risk assessment requires massive validation in order to ensure that the considered phenomena are correctly reproduced. Based on the LNG vapour dispersion experimental database built by ENGIE, a comparative study of various CFD software and models are consequently presented in this article. The first objective is to highlight the positive contribution of CFD together with its current limitations. Special attention is then given to the identification of the current modelling issues to propose further development leads to be undertaken in order to increase the level of accuracy of these tools and overcome their current limitations.

Experimental Campaign

The experimental campaign has been driven by the LNG team of ENGIE Research and Technology Division and took place in May-June 2013, during 3 weeks, on the site of the LNG terminal of Montoir de Bretagne, France, operated by ELENGY.

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The cold LNG vapour generator was designed for generating gas releases for fifteen minutes at temperatures between -110°C and -150°C and controlled flow rate from 2000 to 4000 kg/h. The system, shown in Figure 1, consists in:

- A LNG pressurized mobile tank
- 2 lines with regasifiers, valves and cryogenic tubes
- A mixing box which receives and mixes LNG and natural gas, and releases cold LNG vapour (mainly methane).
- System to control the temperature of the gas release.

- A vent mast at the outlet of mixing box to release cold vapor at a given height and with a given orientation (horizontal or vertical). Two different vent masts diameters were used in order to test different exit velocities with similar mass release rates and temperatures.

Figure 1. LNG vapour generator (left) and LNG vapour release through the vent (right) used during the experimental campaign.

The measuring system is composed of several items:

- A series of movable screens fitted with temperature sensors, and aspirating probes linked to oxygen meters and methane analysers (Figure 2)
- Meteorological station to measure real-time weather conditions during the tests (wind speed at several heights, wind direction, atmospheric conditions etc.)
- Several technologies of imagery were implemented:
    - Infrared cameras: Cooled InSb detector type in the 3.2-3.4 µm spectral range
    - Multispectral imager with 14 channels within the 8 to 14 µm region
    - Hyper-spectral interferometers in the same spectral regions but with higher spectral resolution

Figure 2. movable screens fitted with temperature sensors, and aspirating probes linked to oxygen meters and methane analysers.

Post-processing of measurements allowed to define -amongst 42 tests- 11 time periods in which release and atmospheric conditions are stabilized (atmosphere was neutral in most time periods). For these time periods, set of data needed for dispersion modelling has been extracted (release conditions, wind profiles, gas composition).

The main observation from these tests relies on the physical behaviour of gas plumes which showed that LNG vapour dispersion is very sensitive to wind speed and release velocity, as well as atmospheric condition. Venting with low release velocity and calm atmospheric conditions must be studied very carefully because gas plumes may fall downwards.

Assessment of the Accuracy and Limits of the Different Available Tools

In this part, results obtained with two CFD codes (FLACS and CFX) and with the simple risk assessment software PHAST are compared to experimental results for two release directions (horizontal and vertical) and two vent diameter (6" and 18"). The numerical setup used for each software is based on guidelines and good practices given by software developers. Boundary conditions have been defined based on experimental measures of meteorological conditions. Gas source-terms has been detailed thanks to thermodynamics calculations performed with HYSYS software to estimate the condensation of heavy components occurring in the mixing box and the mass release rate, temperature and composition of released gas at vent exit.

Horizontal 6” diameter release

Input data:

The release is 5,65 m high and 1,4 m downstream from the centre of the mixing box (Figure 3) where a 1.38 m/s wind speed has been recorded. The gas source term has been defined based on HYSYS calculation (Table 1). As first guess, and based on experimental measurement, a ground roughness height of 5 cm has been assumed. Sensitivity to this parameter will be studied in the following.

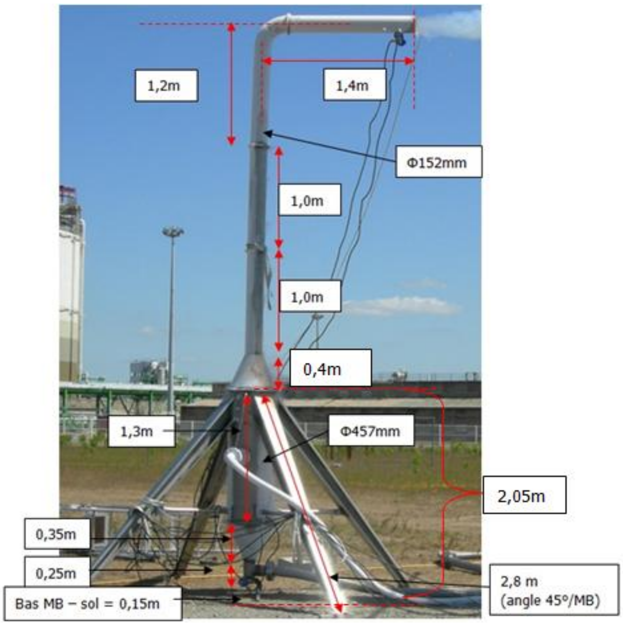

Figure 3. Experimental setup used for Horizontal 6” diameter release.

Gas mass rate (kg/h)	2044
Temperature (°C)	-122.2
%vol CH4	94.82
%vol C2H6	5.0
%vol C3H8	0.14
%vol N2	0.04
Molecular weight (g/mol)	16.79
Density (kg/m3)	1.378
Wind speed at 5.7 m high (m/s)	1.38
Atmospheric stability class	D

Table 1. Input data for Horizontal 6” diameter release.

Results:

Figure 4 shows side views of gas plume, as observed by IR camera (top) and calculated by ANSYS-CFX, FLACS and PHAST. FLACS and CFX give gas plumes similar to the one observed experimentally with a fall down some meters after the release point. On the opposite, PHAST does not predict the fall down of the gas plume and shows a lift-off which can be related to the classic behaviour of a pure methane plume when the gas is initially at ambient temperature. The heavy gas behaviour observed experimentally and numerically with FLACS and CFX is not correctly reproduced by PHAST.

Figure 5 shows gas concentration decay in gas plume calculated by CFX, FLACS and PHAST. Simulations with FLACS and CFX give very good and close results, even if CFX is more conservative than FLACS. FLACS and CFX respectively give a -1% and +20% error on the LFL distance (5%). On the opposite, PHAST overestimates the gas dissipation which leads to underestimated concentrations both in near-field and far-field. This induces 23% underestimated LFL distance with PHAST.

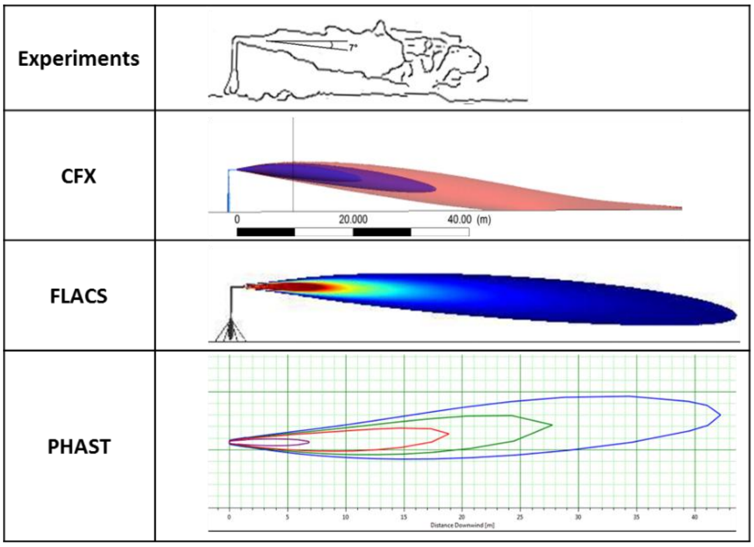

Figure 4. Plume path provided by from top to bottom : experiments (IR cameras), CFX, FLACS and PHAST software - Horizontal 6” diameter release.

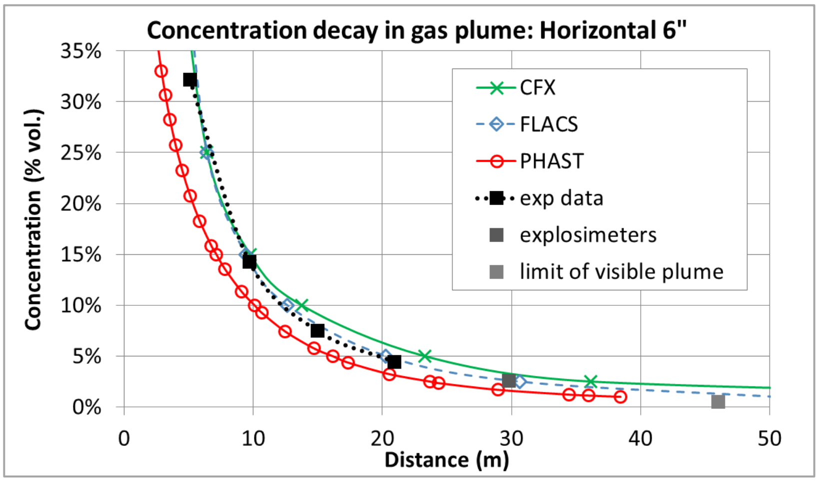

Figure 5. Concentration decay in gas plume - Horizontal 6” diameter release.

Vertical 6” diameter release

<u>Input data</u>:

The release is 4,65 m high and aligned with the centre of the mixing box. A 2.17 m/s wind speed has been recorded at 5.7 m high. The gas source term defined for this case is similar to the 6” horizontal release except for the gas mass flow rate which is 1559 kg/h instead of 2044 kg/h. As first guess, and based on experimental measurement, a ground roughness height of 1 cm has been assumed. If operational conditions from this test slightly differs from the horizontal case, the main difference relies in the release direction which is now transversal to the wind.

<u>Results</u>:

In terms of gas plume (not shown here), results are similar to the 6” horizontal case. FLACS and CFX correctly predict the slow plume fall down observed experimentally whereas PHAST still predicts a rise of the plume.

In terms of hazard distances (Figure 6), FLACS and CFX still give pertinent distances even if CFX is conservative (~ +41% LFL distance). PHAST strongly underestimates the concentration in near-field.

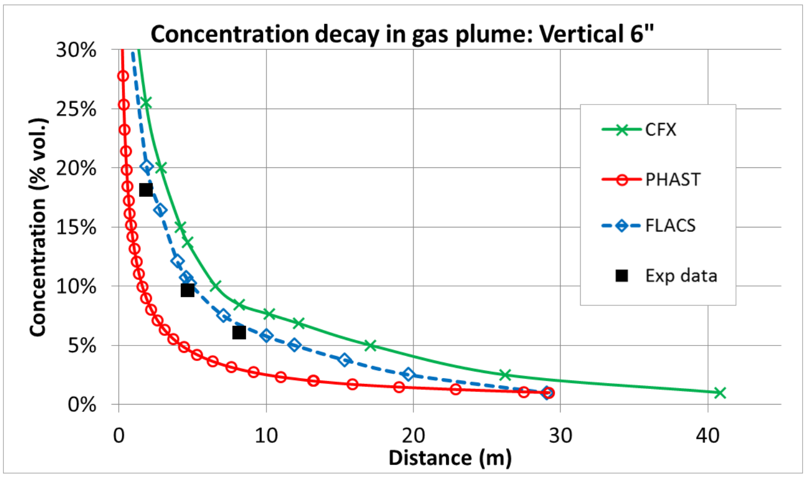

Figure 6. Concentration decay in gas plume - Vertical 6" diameter release.

Vertical 18" diameter release

Input data:

The release is 4,45 m high and aligned with the centre of the mixing box. A 4.73 m/s wind speed has been recorded at 4.15 m high. The gas source term defined for this case is similar to the 6" vertical release except for the gas mass flow rate which is higher : 3687 kg/h instead of 1559 kg/h. As first guess, and based on experimental measurement, a ground roughness height of 3 cm has been assumed.

Results:

Figure 7 shows the plume paths obtained with the different modelling tools. Observations are in line with previous results : Quite similar plume paths are observed with CFD and in experiments. The gas plume modeled by CFX however falls downwards more rapidly than the gas plume modeled by FLACS and appears to be more representative of the experimental observation. PHAST does not predict the fall down of the gas plume.

Figure 8 shows the concentration decay in gas plume, as calculated by FLACS, CFX and PHAST, compared to experimental data. Conclusions obtained here considerably differ from previous results:

- Results obtained with FLACS and CFX are relatively similar (except in very near-filed were FLACS gives lower concentrations than CFX) but tends to underestimate hazard distances both in near-field and far-field: LFL distances obtained with FLACS and CFX are respectively underestimated by around 47% and 31%.
- As previously, PHAST software underestimates the distances in near-field (LFL distance underestimated by around 18%), but appears in agreement with the ½ LFL distance measured by sensors (~1%).

However at this point, these results are insufficient to prove that CFD should be used only for small release diameters and flow rate and that PHAST should be used instead, for far-field.

In order to more clearly assess the limits of the CFD models used or the impact of a potential lack of accuracy of experimental operational conditions, a sensitivity study has consequently been conducted and is presented in next section.

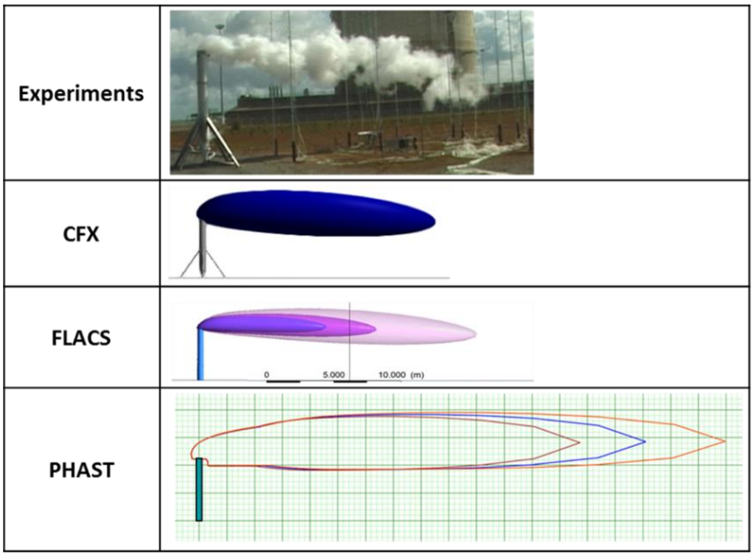

Figure 7. Plume path provided by from top to bottom : experiments (Standard camera), CFX, FLACS and PHAST software – Vertical 18" diameter release.

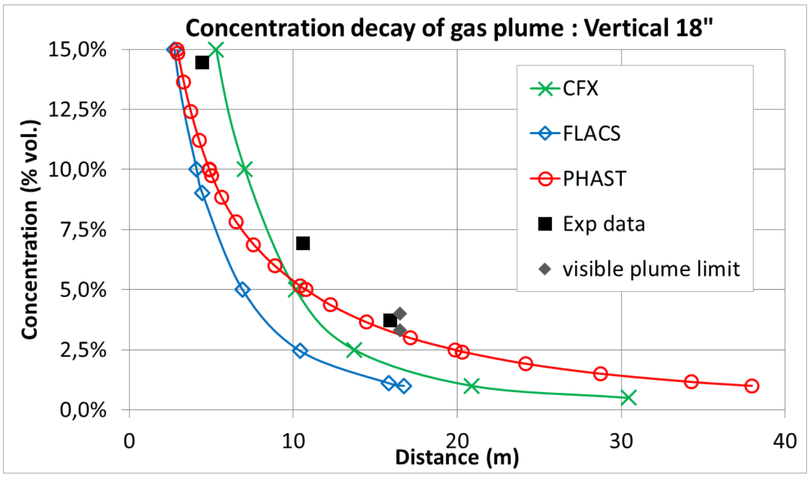

Figure 8. Concentration decay in gas plume - Vertical 18" diameter release.

Sensitivity Study

In this section, the sensitivity of the CFD results to several input parameters and models are evaluated in order to understand either the limits of CFD models or the lack of knowledge of experimental operating conditions which will need special consideration for next experimental campaigns to be conducted.

Sensitivity to ground roughness definition

Up to now, the ground roughness used for simulations have been based on mean wind speed measurements of anemometers. However, from one test to another and even during one test, this quantity can significantly vary, in functions of wind direction in particular. It is clear that the technical impossibility of in situ comprehensive measurement of atmospheric turbulence during tests, brings uncertainties to modelling hypothesis and thus differences on results.

During the vertical 18" diameter release experimental test case considered previously, the ground roughness has been estimated to evolve between 5 mm and 3 cm. FLACS simulations have consequently been performed for each value. Results are shown in Figure 9.

Even with a low value of ground roughness height, FLACS software still underestimates flammable distances (-23% instead of -48% for LFL distance). However, results are considerably impacted by this parameter which requires special attention. Equivalent results have been obtained for CFX and PHAST. In the future, in absence of precise experimental data, it seems consequently more appropriate to define a 5 mm ground roughness in order to ensure a certain conservatism.

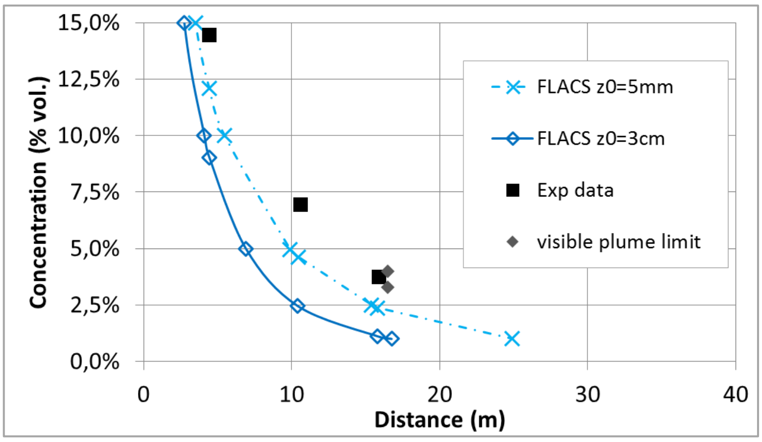

Figure 9. Concentration decay in gas plume - Vertical 18" diameter release – FLACS Sensitivity to ground roughness.

Sensitivity to the definition of meshing at source-term in FLACS

There are two ways to represent gas source-terms in FLACS:

- point sources (each leak located inside a specified grid cell),
- surface area leaks (leaks can cover more than one grid cell, have rectangular or elliptic shape, and one of a given set of spatial source density distributions)

Figure 10 shows the different gas concentration decays obtained with FLACS when using an area leak divided in 4 cells or in 12 cells. A simulation using a point leak has also been performed (not shown here). The tests show that the meshing of the gas source has a significant influence on hazard distances:

- An area leak with 4 cells reduces by 9 to 20% the distances to the different concentrations compared to an area leak with 12 cells.
- A point leak reduces by 27% to 39% the LFL, ½ LFL and 20%LFL distances compared to an area leak with 12 cells.

We consequently recommend to use an area leak with a fine meshing of the gas source (if possible 12 cells or at least 4 cells) instead of point leak. Indeed, it has been observed that the gas source characteristics (exit velocity, gas density) are better reproduced with an area leak.

However, the size of the mesh cells in the area leak must be carefully defined by the modeler: the total surface of the mesh cells located within the "leak box" as defined in FLACS must be equal to the actual area of the gas source). If not, the gas source characteristics can be wrong and the dispersion results too.

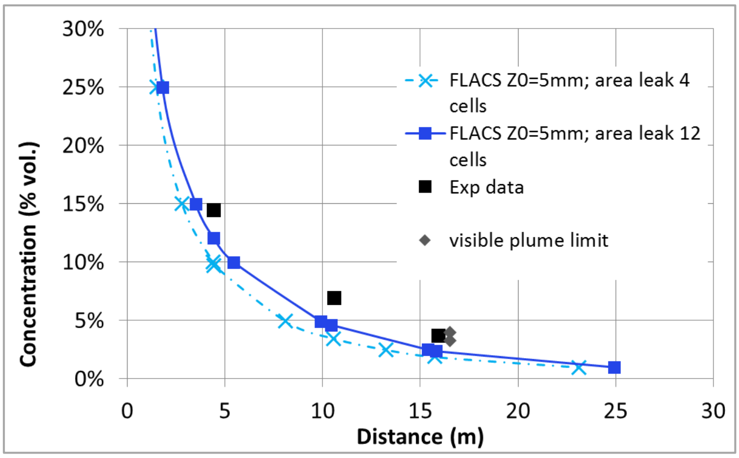

Figure 10. Concentration decay in gas plume - Vertical 18" diameter release – FLACS Sensitivity to the leak source-term.

Sensitivity to turbulence parameters

Figure 11 shows results of CFX simulations with various set of turbulent constants in transport equations. Details of the constants used for each curve are resumed in Table 2.

The buoyancy production term in transport equation for kinetic turbulent energy K (red curve) has a little influence for far-field concentrations (20%LFL distance) is 21.8 m against 21.9 m with no buoyancy terms (green curve).

The buoyancy term in the transport equation for eddy dissipation ε : C3ε appear to have a negligible influence on gas dispersion (orange curve to be compared with the red curve).

On the contrary, the turbulent Schmidt-Prandtl number is influent and decreases the dispersion distances (LFL, ½ LFL and 20% LFL) by 16% when it decreases from 0.9 to 0.7. This parameter seems to be a key factor.

	Curve			
	Blue	**Dark green**	**Orange**	**Red**
Buoyancy production term in transport equation for kinetic turbulent energy K	0	0	1	1
buoyancy term C3ε	0	0	0	1
Turbulent Schmidt-Prandtl number	0.9	0.7	0.9	0.9

Table 2. Constant used for the CFX sensitivity test to constants values.

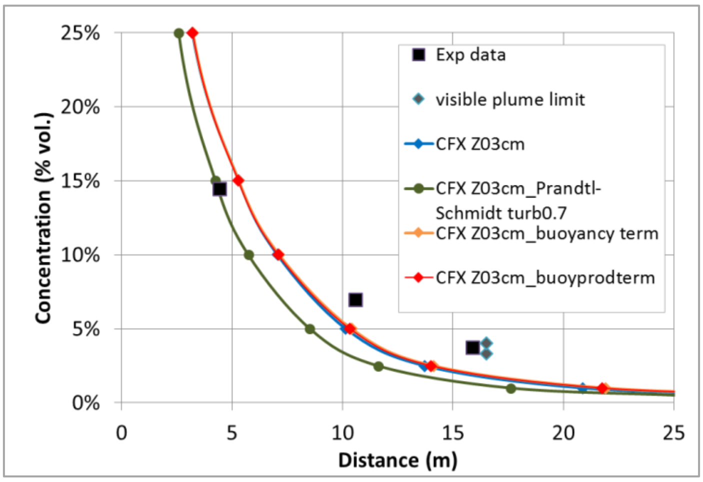

Figure 11. Concentration decay in gas plume - Vertical 18" diameter release – CFX Sensitivity to turbulent model constants.

Sensitivity to wind speed

FLACS simulations on Figure 12 shows that LFL and ½ LFL distances are increased by 15-20% when wind speed at release height is decreased by 1 m/s. LFL and ½ LFL distances are increased by 3-4% when wind speed at release height is decreased by 0,2 m/s (i.e. close to the uncertainty on experimental wind speed measurement). On the contrary, LFL and ½ LFL distances are decreased by 15-20% when wind speed at release height is increased by 1 m/s and decreased by 3-4% when wind speed at release height is increased by 0,2 m/s.

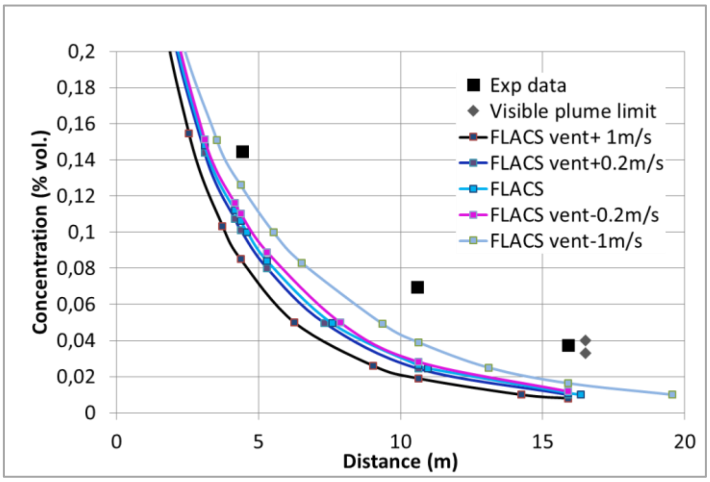

Figure 12. Concentration decay in gas plume - Vertical 18” diameter release – FLACS sensitivity to mean wind speed.

Recommendations And Guidelines For Using Gas Dispersion Models, For Venting Of Heavy And Cold Gases

For the sake of brevity, only a part of available results has been shown here as examples. The recommendations stated here rely on the comparison of CFD software and PHAST results to the full experimental data set retrieved from the campaign performed in 2013 by the ENGIE Lab CRIGEN at Montoir, thanks to funding of ENGIE’s LNG BU and TOTAL.

Conclusions of model/test comparisons and sensitivity studies

The PHAST software appears not to be conservative enough for assessing LFL and ½ LFL distances. The concentration decay on gas plume axis is badly predicted, with bad concentration gradients.

Plume path is badly predicted by PHAST software. In particular, the fall down of gas plume due to gravity effect is not well predicted by PHAST.

Such simple models need more tuning than CFD codes and so need more calibration data with experiments in wind tunnels and outdoor experiments.

The FLACS software shows better results concerning the plume path, but still underestimates LFL distances but above all ½ LFL and 20% LFL distances.

In addition, using FLACS, the modeler must be careful about the implementation of the source-term and the mesh on the source-term. Indeed, FLACS can lead to difference in hazard distances by +/- 100% if the source is badly defined.

The ANSYS-CFX software gives the best results. However, it can appears non conservative, especially for ½ LFL distances and above all for 20%LFL distances which are difficult to predict due to high sensitivity to atmosphere.

But such type of CFD codes (with also Fluent and STARCCM+), with an accurate definition of the source-term appear to be more efficient than CFD tools dedicated to oil & gas safety like FLACS and KFX.

Given the uncertainty on experimental results obtained on very low concentrations (< 2.5%vol), and the large spread of numerical results for such low concentration, It seems very unlikely to be able to calculate 20% LFL distances (used for alarm thresholds on gas sites) in any atmospheric condition with good confidence.

Guidelines

Source-term and meshing in FLACS:

Improvements on source-term definition to be conducted in FLACS software:

There are two ways to represent gas source-terms in FLACS: point sources (each leak located inside a specified grid cell), and surface area leaks (leaks can cover more than one grid cell, have rectangular or elliptic shape, and one of a given set of spatial source density distributions).

CRIGEN carried out a numerical sensitivity study on the definition of the gas source-term and observed quite large discrepancies in the dispersion results between :

- Point source and area source
- Several ways to implement the mesh in area sources

CRIGEN has defined with Gexcon new accurate guidelines to well-define the area sources. This work on source-term meshing in FLACS software will be continued with Gexcon. In addition differences between point leaks and area leaks must be justified and resolved by Gexcon.

CRIGEN recommends to use an area leak with a fine meshing of the gas source of 12 cells (or at least 4 cells) instead of point leak. Indeed, we observed that the gas source characteristics (exit velocity, gas density) are better reproduced with an area leak.

The size of the mesh cells in the area leak must be carefully defined by the modeler: the total surface of the mesh cells located within the "leak box" as defined in FLACS must be equal to the actual area of the gas source. If not, the gas source characteristics can be wrong and the dispersion results too.

Outside of the source-term, CRIGEN recommends to strictly follow the grid guidelines given by Gexcon, i.e a maximum size of cell is 1 m at the boundaries of the calculation domain, and stretch ratios in X, Y and Z directions lower than 1,1.

Turbulence level at source-term is not so influent provided it is imposed at standard level : CRIGEN recommends to select a turbulent intensity of 5% and a turbulent length of 15% of the diameter of the vent exit. This is also verified for ANSYS-CFX code.

Source-term and meshing in CFX (it can be transposed to similar codes : Fluent and STARCCM+):

CRIGEN recommends to use an adaptative mesh, function of gas concentration gradients, which is very efficient to solve properly the gradients of the flow. The size of the cell shall vary from 5 mm close to the vent exit to 1 m for extreme zones of the calculation domain where there is no gas species to be tracked.

Physical hypothesis:

- For all models, it is necessary to assume a low ground roughness height as input because :
    - It appears that available standards on the choice of ground roughness heights functions of environment overestimate the ground roughness heights (when comparing with measurement campaigns)
    - Ground roughness heights is changing functions of wind direction but also functions of the season, and measurements campaigns showed that the variation can be very important (from 1 to 10).
    - Comparisons of simulations with our experimental campaign show that when using a low ground roughness height (lower than 1 cm or 5 mm), results are closer to measurements.

    ⇨ CRIGEN recommends not using a ground roughness height upper than 5 mm.
- Mean wind speed has the more important influence on hazard distances after the ground roughness height. In any case, one should not overestimate the wind speed to select in the model calculations, because the lower the wind speed, the higher the hazard distances.

    ⇨ CRIGEN recommends not using mean wind speed but a wind speed representative of low wind period, e.g night conditions with stable atmosphere. The low wind speed used for simulations shall be based on wind statistics.

Model parameters:

- Using a turbulent Prandtl-Schmidt number of 0.9 (default value in CFX) instead of 0.7 in the CFD model increases the hazard distances by 10-20%, which is more in agreement with the experimental data we get.

    ⇨ CRIGEN recommends using a turbulent Prandtl-Schmidt number of 0.9
- In our simulations, we does not observe large influence of buoyancy terms to be implemented in K transport equation and in ε transport equation (> 10%).

    ⇨ However, CRIGEN recommends implanting a buoyancy production term in K transport equation Pkb and a C3ε constant equal to 1 (C3ε is implemented in ε transport equation). Appendix 3 gives more information on these parameters.

General recommendations about software to use

Based on our results and our understanding of the weakness of different numerical tools which have been tested, we advise – when possible – to use ANSYS-CFX tool, or a similar CFD code (Fluent or STARCCM+) which use a refined mesh and numerical scheme – after comparisons with ANSYS-CFX code –.

Using such a tool implies modelling difficulties.

- First, the mesh is finer than in FLACS, and so there are more cells, and the calculation time is higher. However, these codes provides unstructured mesh unlike FLACS which uses a Cartesian cubical structured mesh. In consequence, it is possible to refine mesh in gradient zones and stretch the mesh where there is no relevant physics. In addition, CRIGEN has tested with success in CFX an adaptative meshing tool which optimizes automatically the mesh size.
- Second, one of the major advantages of the tools dedicated to oil and gas safey like FLACS (or KFX) is that they provide a tool to automatically build a mesh on a site geometry from a 3D CAD model. This allows to run simulations on very large site, quickly.

CFX and STARCCM+ provide tools which can help the modeller to build a mesh from a geometry site, but it is not so easy and quick. However, CRIGEN is working on this issue with CFX, and some engineering companies have also worked on it and they can already use CFD codes like STRACCM+, CFX or FLUENT with a large geometry of a site.

Perspectives

There are still uncertainties on the validity of models for low momentum cold/heavy gas releases, even for CFX code which appears to be the more valuable approach tested by CRIGEN. Models can appear non-conservative, especially for low concentrations (< 5% vol).

Indeed, the issue of atmospheric dispersion of low momentum cold/heavy gas releases is complex, due to strong influence of atmospheric turbulence which is hard to model in industrial sites.

Further R&D studies, with wind tunnel experiments and comparisons of "standard" models with more advanced CFD codes like Large Eddy Simulation (LES) codes are highly recommended (CRIGEN is currently set up a partnership to do so).

In parallel we recommend to develop the knowledge on CFD modeling, with commercial multi-application tools like CFX, FLUENT or STARCCM+.

CFD tools dedicated to oil and gas safety like FLACS and KFX and simple models like PHAST have shown their limits on atmospheric dispersion of low momentum cold/heavy gas releases.

Several engineering companies have already changed their practices by using STARCCM+ instead of FLACS for ventilation and dispersion studies in offshore applications.

Finally, CRIGEN can also develop and propose in EVOLCODE software a simple model for simulating quickly heavy/cold gas venting (without obstacle). This model could be calibrated with Montoir 2013 experiments and CFX simulations. And it could provide quick results with more confidence than PHAST software which showed strong limitations.

References

Sail, J., Blanchetière, V. & Giacosa, A., 2015. *LNG vapor dispersion test campaign to qualify spectral cameras and dispersion models. GASTECH* Singapore.