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Gas Dispersion Simulations By Means Of The Kfx Code

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Simplified models (Gaussian and Integral Models) have been traditionally used in environmental and hazard evaluations for dispersion scenarios. They have generally undergone an extensive deal of validation against experimental data and, as a consequence, they are believed to provide acceptable accuracy at least for conditions covered by the experimental range. On the other hand, CFD models - applied to dispersion scenarios - do not still exhibit the same comprehensive record of validation work as for simplified models.
In this work the sensitivity of the Kameleon FireEx (KFX) CFD code to some geometric and numerical parameters has been assessed in order to single out parameters that mainly drive the numerical results deserving particular care in their assignment.
Results have shown that for the ranges of cell size and time step adopted, numerical calculations are mostly sensitive to the levels of atmospheric turbulence intensity.

1. Introduction

Due to the importance of a sound estimation of dispersion scenarios, many models have been developed during years following quite diverse approaches (Lees,1996). Proposed models range - in terms of increasing complexity - from Gaussian models to fully 3-D CFD models the Integral Models standing as a trade-off between these.
Since Gaussian and Integral Models have been traditionally used in evaluations of hazardous consequences, they have also undergone an extensive deal of validation against experimental data (Lees, 1996). As a consequence, they are believed to provide acceptable accuracy at least for conditions covered by the experimental range.
The breakdown of such simplified models occurs unavoidably when geometry becomes an issue. Gaussian and Integral models are not able to properly take into account realistic geometries in terms of terrain complexity (non flatness) and, most importantly, in terms of obstacles such as buildings and/or congested industrial environments. In such conditions, CFD models turn to be the only suitable option, due to their natural ability to allow for boundary conditions of whatever complexity.
On the other hand, CFD models do not still exhibit the same comprehensive record of validation work as for simplified models. Several works have recently appeared aimed at assessing the capability of CFD codes in reproducing experimental data for gas dispersion scenarios (Riddle et al., 2004; Hanna et al., 2004; Sklavounos and Rigas, 2006; Scargiali et al., 2004). All have claimed the aptitude of CFD codes in predicting the main characters of the physics of the problem still standing uncertainties in the quantitative side.

Work is currently ongoing at Snamprogetti to thoroughly assess the Kameleon-FireEx CFD code against experimental field data for gas dispersion scenarios. A prerequisite of such work was an assessment of the code sensitivity to some geometric and numerical parameters. When comparing experimental and numerical data, care must be taken to ascertain whether possible differences are to be ascribed to modelling choices or numerical issues (grid size and time step). To this aim it appears of paramount importance to find out proper cell size and time step amplitude that do not grossly affect the numerical results.

2. Aim of the work

The aim of the work is to present the results of the sensitivity study carried out for the commercial CFD code Kameleon-FireEx.
The code was assessed in terms of an accidental gas release in a simple geometry (plume from an elevated continuous release on a flat surface representing the sea surface). The scenario under consideration stems from real operating conditions in a off-shore installation. No experimental data were available for such scenario.
Table 1 summarizes the operating conditions of the item undergoing the accidental leak together with the wind conditions and the geometric characteristics of the release. The actual fuel is a complex multi-component mixture (comprising Hydrogen Sulfide H_2S) that was assimilated to a pure compound with an equivalent molecular weight (i.e. the average molecular weight of the actual mixture). The total mass flow rate ensuing from the leak was some 12 kg/s with a 23% H_2S content.

Table 1 – Release scenario

Stream operating Conditions		Wind conditions		Release characteristics	
Temperature, K	430	Velocity, m/s	10	Hole size, m	0.022
Pressure, bar a	95	Category	*D*	Height of release, m	15
Molecular Weight	26.22	Temperature, K	283	Angle with the ground, °	0

Figure 1 shows the calculation domain that was set up exploiting the symmetry of the problem. A symmetry plane was considered cutting half the release along the *x*-axis.
The physical dimensions considered were: L_x=500m, L_y=80m, L_z=100m and were considered to be large enough to prevent any influence of the boundary conditions on the flow calculation.

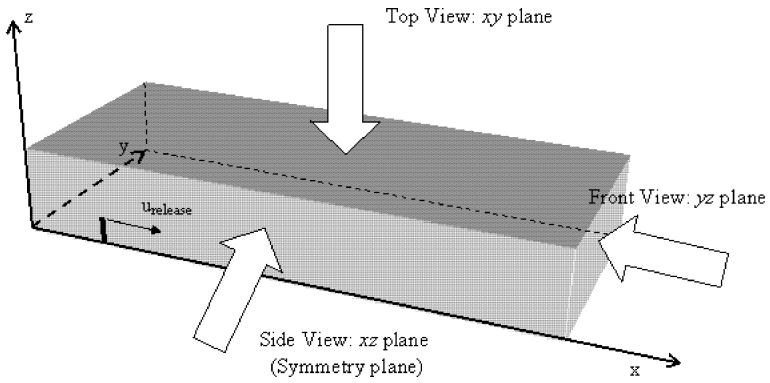

Figure 1 – The calculation domain displaying the symmetry plane.

3. The tool

Kameleon FireEX is a CFD commercial code developed by the Norwegian Compute IT (Magnussen et al., 2000) specifically oriented toward dispersion and fire scenarios. It is a cartesian, incompressible, Finite Volume CFD code that solves the discretized conservation equations for mass, energy and momentum adopting an iterative implicit pressure-correction method.

4. Effect of varying parameters

Both numerical parameters - grid density and time step size - and model parameters - such as the source term and turbulence levels in the boundary conditions - were investigated. The study was carried out by varying one parameter while keeping constant the others.

4.1 Effect of grid refinement

Grid density and topology are usually crucial parameters in determining the numerical solutions of a discretized system of equations. Good practice in CFD calculations demands a systematic appraisal of variations of the numerical solutions as a function of the cell size. Grid refinement should be systematic i.e. the cell size should be gradually decreased - or increased - by halving or doubling it till at least three solutions are gained on three different grids (Ferziger and Peric, 2002).

In this work we did not aim at an estimation of the numerical error and considered just two grids. The two grids are shown in Figure 2. By looking at the H_2S concentration along the downstream distance, it can be seen that results are very close for the two grid densities (see Figure 3).

4.2 Effect of the time step

KFX adopts an implicit resolution method so that stability of solutions is always ensured (the algorithm is said to be *unconditionally stable*). A proper choice of the time step is however necessary in order to accomplish accuracy of solutions.

Simulations were run with two different Courant Numbers (1 and 10) respectively carrying two different maximum time steps (3.7×10^{-3} and 3.7×10^{-2} s). The transient

build-up of the H_2S concentration were practically overlapped ensuring that a relatively large time step (10^{-2} s) is satisfactorily accurate.

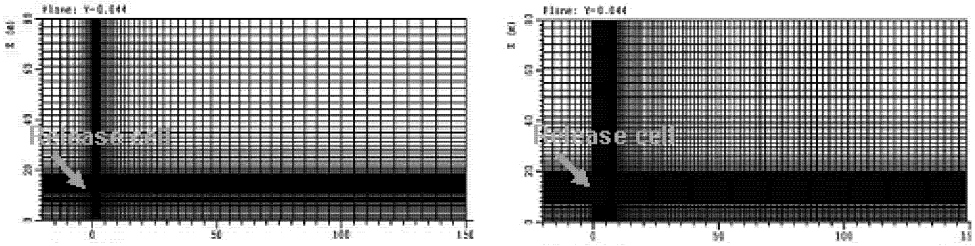

Figure 2 – Grid refinement: *xz* plane. The grid on the left side of the picture has 345920 cells (115x47x64) the one on the right part has 1060101 cells (213x63x79).

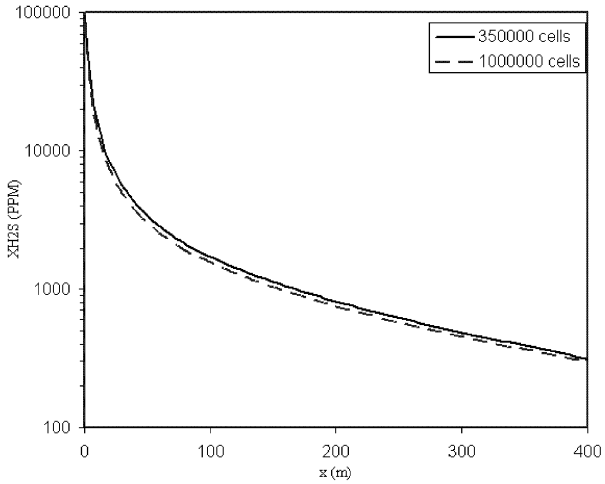

Figure 3 – Grid effect: comparison between numerical results for 350000 cells and 1000000 cells. Concentration profiles for H_2S along the downwind distance (*x*-axis) at *z*=15m (the height of the release).

4.3 Effect of the source term

The high pressure level in the leaking item (P=95 bar), originates a supersonic jet. The structure of such a jet is very complex and it would require a fully compressible code to be described. Also, due to the fine structure of a shock wave (the variables abruptly change across a distance of few molecular paths), the whole computational budget (around 10^6 cells) would be required for the near field description of the release.

Suitable sub-models are usually employed that yield equivalent values for the velocity, the concentration and the jet section downstream of the release where low Mach number have been restored and the incompressible assumption turns acceptable.

Simulations were run with the KFX code with two different such submodels and, again, the difference was not really significative. The two submodels were respectively the one available in KFX and the one available in the HGSYSTEM integral model. They both solve the one-dimensional conservation equations for the supersonic stream ensuing from the hole. They basically differ for the downstream distance where "equivalent" variables are evaluated (i.e. the distance where atmospheric pressure and incompressibility have been restored). On the left side of Figure 4 is reported the "concentrated release": u=359 m/s; y_{fuel} = 0.545; D_{eq}=0.176m; on the right side the "distributed source": u=58.3m/s, y_{fuel} =0.09; D_{eq}=0.886m; u is the x-component of velocity, y_{fuel} is the mass fraction of the equivalent fuel and D_{eq} is the equivalent diameter of the expanded jet.

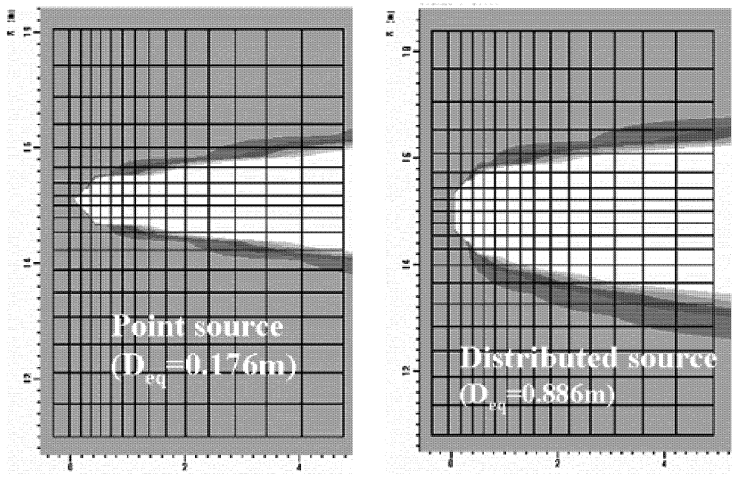

Figure 4 – Effect of the source term. Details of the two source terms.

4.4 Effect of the turbulent intensity in the Boundary Conditions

The atmospheric turbulence levels depends on the heat fluxes promoted by vertical temperature gradients. KFX does not simulate the vertical temperature profile so that the generation of atmospheric turbulence must be modelled.

As many other codes, KFX determines the intensity of the atmospheric turbulence by means of a parametrization of the Pasquill stability classes. In other words, each stability class is assigned a numerical value of the turbulence intensity.

Simulations were run for three different values of the turbulence intensity (I = 0.07, 0.14, 0.21) and results are shown in Figure 5. It can be seen that the turbulence intensity is undoubtedly the most crucial parameter in affecting the dispersion of the H_2S. Its influence is particularly important in the far field where a passive dispersion mechanism has definitely established and atmospheric turbulence is solely responsible for the H_2S dispersion.

5. Conclusions

The KFX code was assessed in terms of its sensitivity to numerical and modelling parameters. The code proved quite robust in terms of varying numerical parameters as

the grid resolution and the time step. On the other hand, it resulted quite sensitive to the turbulence intensity assigned on the boundary conditions. The latter finding appears quite interesting standing the acknowledged tendency of many CFD codes to underestimate turbulence (Dharmavaran et al., 2005) in the Atmospheric Boundary Layer. Such underestimation is deemed to originate from:

1) poor parametrization of stability classes

2) lack of modelling of low frequency atmospheric motions ("atmospheric meandering").

Bearing in mind the sensitivity of the KFX code to turbulence intensity and the weakness of many CFD codes in correctly describing the Atmospheric Boundary Layer, it is here endorsed the necessity of a full appraisal of the stability classes parametrization adopted in KFX.

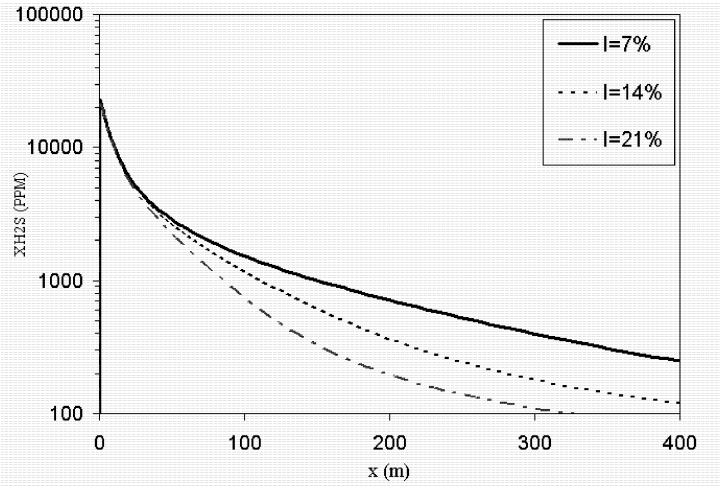

Figure 5 – Effect of the turbulence intensity in the Boundary Conditions. Concentration profiles for H_2S along the downwind distance (x-axis) at z=15m.

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