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Modelling of Vented Gas Explosions in the CFD tool FLACS

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Accidental explosions occurring in enclosures can be efficiently mitigated by installing pressure relief panels. The venting process enables the combustion products to expand without subjecting the main structure to destructive overpressures. However, the pressure development in time will be the result of several physical phenomena, interacting in different ways depending on parameters such as the vent size, the ignition position, the panel opening pressure, the vent panel mass per unit area, the presence of obstacles, the layout of the chamber, and the combustion properties of the fuel. Due to the complexity of the problem, it is difficult to produce one universal venting guideline for all cases.
In principle, detailed CFD (Computational Fluid Dynamics) simulations should allow for the representation of all physical processes affecting vented explosions, thus allowing for a consistent prediction of the expected overpressure loads. A series of experiments performed at FM Global (Bauwens et al., 2010) have been simulated using the CFD tool FLACS. The results show that some of the pressure generating mechanisms are represented well, while others are not modelled properly. The relevance of representing each phenomenon for the final application of FLACS is discussed.

1. Introduction

The production, handling, transport, and usage of large quantities of flammable gas and liquids in the petrochemical industry require adequate means for the prediction of the consequences of potential accidental gas explosions. The reliable prediction of overpressure loads resulting from such explosions can allow the planning of realistic and optimum safety measures. Explosion venting is commonly used in the process industry as a loss prevention solution to protect equipment or buildings against excessive internal pressures caused by the explosion. It involves the use of "vents" that "yield" when the overpressure following an explosion exceeds a certain value, and the resulting pressure relief ensures that the maximum overpressure does not exceed the design load.
The subject of vented explosions has been widely studied, both experimentally as well as numerically. Both laboratory-scale (Cooper et al., 1986) and large-scale experiments (van Wingerden, 1989) have been carried out. Analytical models and empirical correlations have also been developed (Bradley and Mitcheson, 1978). Engineering guidelines and standards such as EN 14994 (CEN, 2007) have been made based on some of these correlations. However, the guidelines often have conflicting recommendations due to the number of different factors that may influence the peak overpressure.
Recently, FM Global have carried out a series of experiments to study the effect of ignition location, vent size and the presence of obstacles in a series of vented near-stoichiometric propane-air explosions performed in a 64 m^3 chamber without a pressure relief panel (Bauwens et al., 2010). A total of three pressure peaks were observed. The first peak is caused by the external explosion that

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follows the ignition of the vented unburned gas, involving Rayleigh-Taylor instabilities and Helmholtz oscillations. With back ignition, the effect of the external explosion dominates, since a larger amount of unburned gas is pushed outside the chamber before it is ignited. Bauwens et al. (2010) call this peak P1. The pressure peak occurring after P1, corresponding to the time when acoustic waves enhance the area of the flame, is denoted P2. This peak gets increasingly important as the distance between the ignition point and the vent opening decreases. The insertion of eight square obstacles introduces a third distinct peak, P3, corresponding to the time when the maximum flame area is reached inside the chamber, normally occurring after P1 - but before P2 (see Figure 2, left). The presence of obstacles significantly dampens the magnitude of P2. A reduction of the vent area increases the magnitude of all pressure peaks.
In the following, the ability of the CFD code FLACS to reproduce experimental results obtained in a selection of these vented explosion vessels – with and without obstructions – is addressed. The representation of the various mechanisms that result in the observed overpressure profiles is emphasised.

2. The CFD-tool FLACS

The simulations reported in this study have been carried out using the CFD tool FLACS, version 9.1, release 3 (GexCon, 2010). The FLACS code is primarily aimed at simulating the dispersion of flammable gas in process areas, and subsequent explosions of gas-air mixtures. Significant experimental validation activities have contributed to the wide acceptance of FLACS as a reliable tool for the prediction of natural gas explosions in real process areas both offshore and onshore. FLACS solves the compressible Navier-Stokes equations on a 3-D Cartesian grid using a finite volume method. The conservation equations for mass, momentum, enthalpy, turbulence and species, closed by the ideal gas law are included (Hjertager, 1986). The FLACS code uses a “distributed porosity concept” which allows the representation of complex geometries using a Cartesian grid. Large objects and walls are represented on-grid, sub-grid objects result in partially blocked control volumes, given by the computed porosity value. FLACS uses a standard k-ε model (Launder and Spalding, 1974) for turbulence. However, several important modifications are implemented, including a model for turbulence generation behind sub-grid objects (Arntzen, 1998).
FLACS contains a combustion model that assumes that the flame in an explosion can be regarded as a collection of flamelets. One-step reaction kinetics is assumed, with the laminar burning velocity being a measure of the reactivity of a given mixture. The flame model gives the flame a constant flame thickness of 3-5 grid cells and ensures that the flame propagates into the reactant with the specified velocity that accounts, among others, for the flame wrinkling due to instabilities and turbulence levels.

3. Brief Description of the FM Global Experimental Setup

The experimental data used here for the validation of the CFD tool FLACS were obtained by FM Global in a 64 m^3 explosion test chamber with overall dimensions of 4.6 × 3.0 × 4.6 m^3 in a series of experimental tests. The chamber had a square vent of either 5.4 m2 or 2.7 m^2 located on the front wall, corresponding to either 39 % or 19.5 % of the total front wall area. Four pressure transducers were mounted on the chamber walls to measure the pressure-time data. Three different ignition locations were used in the experiments: at the centre of the chamber (centre ignition), 0.25 m from the centre of the wall opposite the vent (back-wall ignition), or 0.25 m from the centre of the vent (front-wall ignition). For tests performed with obstacles, eight 0.40 × 0.40 m^2 square obstacles spanning the full height of the chamber were uniformly distributed in two rows of four with 0.75 m of spacing between obstacles. A view of the experimental setup including obstacles is presented in Figure 1. An overview of the experimental configurations is given in Table 1. More details can be found in (Bauwens et al., 2010).

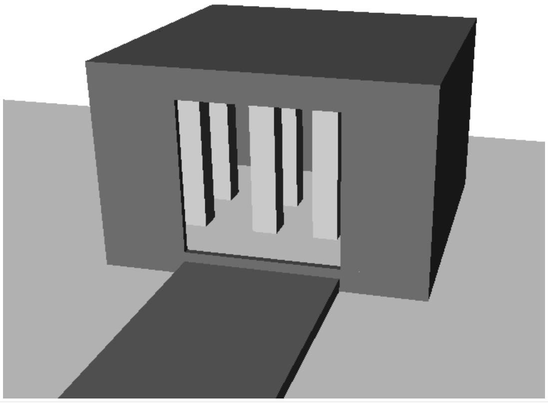

Table 1: Ignition positions in the different configurations of the experiments

Vent size (m^2)	No obstacles	8 obstacles
2.73	Back Centre Front	 Centre Front
5.43	Back Centre Front	Back Centre Front

Figure 1: A view of the experimental setup as represented in the simulations.

4. Results and Discussion

The experimental uncertainty associated with P1 and P3 is 25 %, as described by Bauwens et al. (2010). The pressure peak P2 shows some more variability – for one particular case, there was a discrepancy range of ± 50 % for the maximum overpressure for repeated tests. To the authors' knowledge, the uncertainties are acceptable for use in this study.

All the FLACS simulations were run with two grid resolutions: 0.20 m and 0.10 m. The grid dependency was generally found to be acceptable, see Figure 2 (left), so the coarser grid resolution was used for the general analysis.

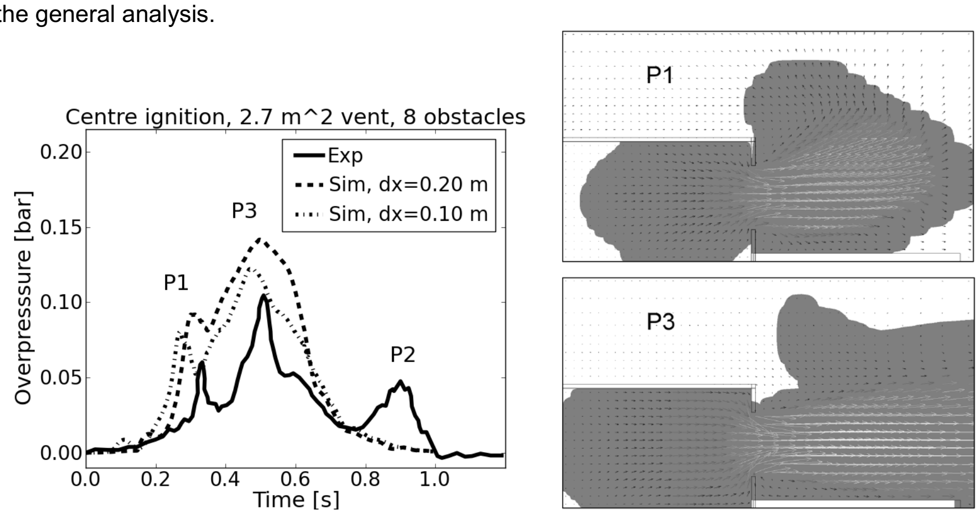

Figure 2: (left) Pressure development in time for grid resolutions of 0.10 m and 0.20 m for 4 vol% propane-air. (right) Burnt gas at the time of the pressure peaks for 4 vol% propane-air.

Bauwens et al. (2010) report an initial turbulent velocity fluctuation of 0.1 m/s in the fuel-air mixture, but no information about the initial dissipation is given. Initial turbulence was therefore also assumed in FLACS. This is a potential source of uncertainty for the simulated results, since turbulent flow can significantly enhance the rate of combustion. In the FLACS simulations presented here, a sensitivity study was performed to reveal the effect of adjusting the initial turbulence level and reasonable values (a turbulent velocity fluctuation of 0.1 m/s and an initial turbulence length scale of 0.01 m) were applied consistently throughout the whole analysis.

Figure 2 (right) presents the burnt products of the explosion at the time of the pressure peaks P1 and P3 showing the flame location when these peaks are observed. Figure 3 shows the effect of obstacles on the explosion overpressures. The overpressures are higher when eight obstacles are present, since the turbulence generated when the flow interacts with the obstructions enhances the combustion. A comparison of the experimental observations and simulations for the pressure peaks denoted by P1 and P3 for propane-air explosions is presented in Figure 4. The figure includes results for all configurations for which the experimental value of the pressure peak in question is reported by Bauwens et al. The limits of ± 30 % for under- and over-prediction of the experimental values are considered to be reasonable for studies of this nature.

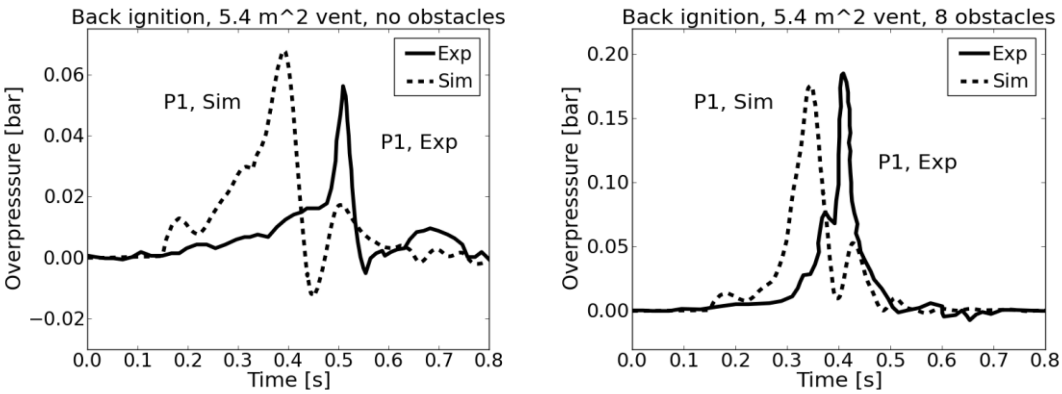

Figure 3: Explosion overpressure as a function of time for 4 vol% propane in air with back ignition and a 5.4 m^2 vent opening, (left) no obstacles, (right) eight obstacles.

According to Bauwens et al. (2010), the first pressure peak (P1) is associated with the external explosion, Helmholtz oscillations and Taylor instabilities. The reactivity of the fuel will also play a role here (Cooper et al., 1986). FLACS represents the amplitude of this pressure peak well, as presented in Figure 2 (left) and Figure 3 (left and right). In Figure 3, the pressure build-up starts earlier for the simulated results, but the general shape of the dominant peak is reproduced. The oscillations that can be seen in the FLACS results after P1 in Figure 3 (left) may be more pronounced than for the experiment because of dampening factors not present in FLACS (e.g. structural effects). The over-prediction of the smaller pressures (as observed in Figure 3, left) becomes less significant with an increase in scale, due to the sub-grid modelling of turbulence and combustion. As the simulated flame has a constant thickness of 3-5 grid cells, grid dependency cannot be completely avoided.

The second pressure peak in Figure 2 (left), called P3, corresponds to the time when the maximum flame area is achieved in the chamber. This is only discernible in the experiments with obstructions. In the experiments with back ignition, P1 and P3 are coupled. In Figure 3 (right), the time of maximum flame area is achieved in FLACS slightly after P1, so here, the pressure peaks are separated. However, the dominant peak is well reproduced.

The pressure peak associated with the acoustics effects (P2) is not reproduced by FLACS, see Figure 5. This peak is caused by the interaction of the flame and pressure waves travelling back and forth within the chamber, thus leading to higher burning rate and magnification of the pressure amplitude. These effects are not modelled in FLACS. Consequently, when acoustic effects dramatically dominate the overpressures (for front ignition, and to some extent central ignition – mainly for empty enclosures with small vent openings) FLACS may under-predict the pressure values. A correct representation of this phenomenon would require a higher resolution in space and time, and a coupling between the reactive flow and the structural response of the chamber.

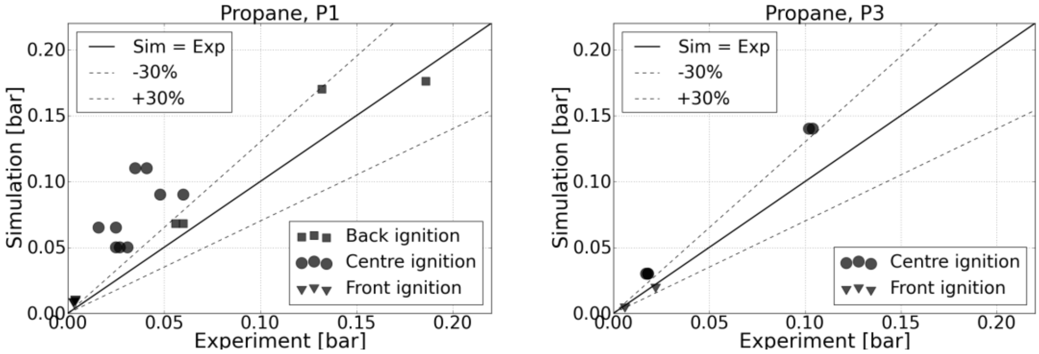

Figure 4: Experimental vs. simulated results for overpressure peaks P1 (left) and P3 (right) for all configurations. A gas mixture of 4 vol% propane in air was used for all simulations.

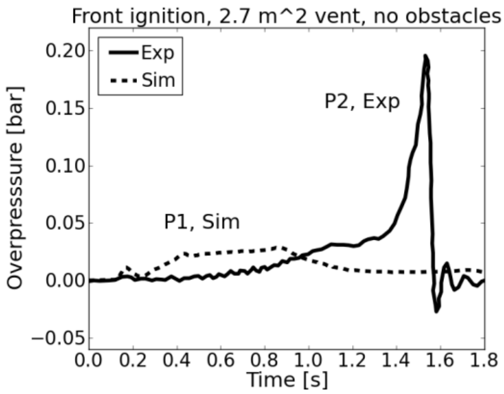

Figure 5: Pressure as a function of time with front ignition and a 2.7 m^2 vent opening (4 vol% propane-air). The peak P2 is due to acoustic effects – not represented in the simulations.

Another potential source of uncertainty is the use of the k-ε model. Despite its known limitations, it is a powerful model for industrial applications. The use of this model inside FLACS is well validated and reasonably robust. With the close coupling between sub-grid modelling and turbulence model, it is not certain that replacing it with a more advanced turbulence model will give much added value. Nonetheless, testing of alternative turbulence models will be a part of the future FLACS development.

A series of methane explosions with a corresponding experimental setup (Chao et al., 2011) were also simulated, see Figure 6. The FLACS results for pressure peaks P1 and P3 are generally within the ± 30 % limits of discrepancy with the experimental data, and are therefore considered to be satisfactory.

5. Final Remarks

FLACS CFD simulations of the vented explosion experiments carried out by FM Global in their 64 m^3 chamber have been performed and analysed. The simulation results are compared to the experimental data for several experimental configurations for both methane and propane, including two different vent areas and three different ignition locations.

The simulations seem to agree reasonably well with the experiments, and may be used for estimating pressure loads for vented explosions. The results are considered to be satisfactory when the peak overpressure and duration is in reasonable agreement with the experimental values. In addition, the pressure peak should be caused by the appropriate physical mechanism. Where there are significant discrepancies for P1 and P3, the results are in general conservative. FLACS may under-predict the overpressure in situations where the acoustic effects (represented by P2) dominate. However, P2 is significantly damped when obstacles or irregular surfaces are present (Cooper et al., 1986), as they will be in most practical situations.

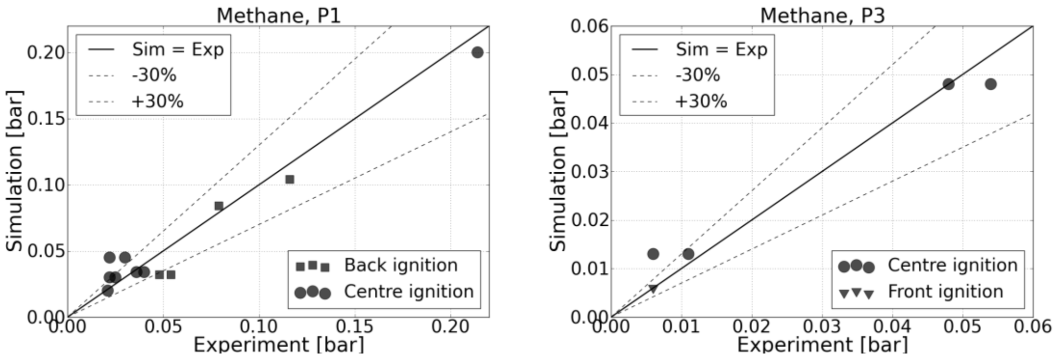

Figure 6: Experimental (Chao et al., 2011) vs. simulated results for overpressure peaks P1 (left) and P3 (right) for all configurations. A gas mixture of 9.5 vol % methane in air is used for all simulations.

Acknowledgements

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