CFD Modelling of Mist Explosions Experiments

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1 Introduction

In the process industries, combustible gases and liquids are typically stored and transported at elevated pressures, and accidental loss of containment may result in formation of flammable fuel-air clouds. Whereas dispersion and combustion of gaseous fuels have been investigated extensively in the past [1-3], less work has been done on liquid releases [4-5] and 'premixed combustion with non-premixed substructures' [6-7]. However, several major accidents have involved mists, including Buncefield [8] in the petroleum industry and the hydroelectric power plant Roncovalgrande [9].

Validation against large scale dispersion and explosion experiments confirms that CFD tools can predict the development of gas clouds and explosion loads with reasonable accuracy. However, only a limited number of tests have been done concerning generation, ignitability and combustion of aerosol clouds and few models has been implemented in CFD codes.

The present work focuses on experiments that were done in order to gain a better understanding of aerosol explosions in general and to investigate the performance of FLACS in simulating such phenomena. Aerosols, or clouds of liquid droplets in air, are mainly formed through two processes [10]: atomization of a liquid (spray) or condensation of saturated vapour (mist). A distinction is made between mists and sprays with respect to droplet size distribution: the droplets in a mist are generally smaller than those in a spray. The droplet size is of primary concern with respect to safety, since it determines how the flame propagates through the cloud, and hence the violence of the explosion.

2 Description of the selected experiments

This section describes experiments involving aerosol explosions. In both cases, the aerosol clouds were created by the atomization of a liquid in the form of a spray.

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The first experiment has been performed during the joint industry project "Limitation of the Consequences of Release of Flammable Substances" (LICOREFLA) from 2000 to 2002 [11]. The tests were carried out in a 2.5m x 0.3m x 0.3m channel. Two "square orifice" baffles, with a blockage ratio of 50%, at x=0.39m and x=1.33m, were used to accelerate flames and increase flow speed locally to enhance droplet break-up. They were used in two configurations: both baffles or only the one at 0.39m. A 47% baffle plate was also mounted at the end of the channel. Its role was to slow down the venting, so that higher pressures and differences between the different oil mist explosions could be measured. The ignition source was an electrical spark discharge, located centrally at the closed end of the channel (x=0). The first 0.5m of the channel were filled with a lean propane-air mixture (2.86 vol % propane in air corresponding to an equivalence ratio ER of 0.7). Combustion of this mixture initiated the oil mist explosions. This approach resulted in a repeatable initiating flame with limiting influence on the flame propagation through the mist in the downstream parts of the channel.
Four piezoelectric pressure transducers from Kistler were used to measure the transient pressure. These were located at x=0.25, 1.04, 1.64 and 2.44m. The test setup is shown in Figure 1.

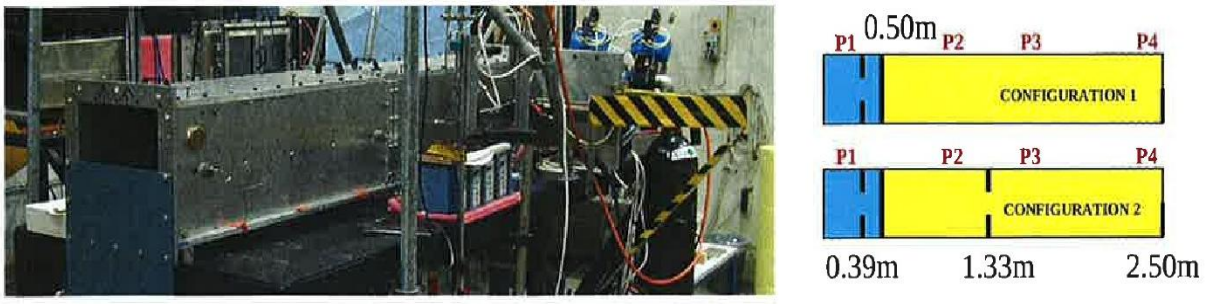

Figure 1. Test rig with baffles configurations on the right. Blue section represents the lean propane, the yellow one the oil mists from sprays.

Three different types of oil were used in the experiments: hexane (C_6H_{14}) was used to represent a flammable liquid with flashpoint below room temperature, decane ($C_{10}H_{22}$) represented high flashpoint flammable liquids and low sulphur crude oil from the North Sea (Oseberg blend) was included as an example of a real industrial application. Particle size measurements mist with a Malvern indicated a Sauter Mean Diameter (SMD) in the range 10-15µm for the droplets. However, it is unclear if the SMD was conserved when the oil was dispersed into the rig. No *in-situ* measurements were made to confirm this. It was assumed that the diameter was maintained but the Malvern measurements were performed in open space while the rig is a confined space, which means that some interactions between droplets have been neglected.

Table 1 summarizes the ER investigated for the various types of oil. The ER values in the table assume complete combustion in air of all the oil, and not the actual ER during combustion reactions. No measurements of ER were performed in the rig.

ER (Equivalence Ratio)	Hexane - Total oil quantity (ml)	Decane - Total oil quantity (ml)	Oseberg blend - Total oil quantity (ml)
0.5	10.22		
1.0	20.44	18.83	13.84
2.0	40.88	37.66	27.68
3.0	61.32	56.49	41.52
4.0	81.76		

Table 1 Oil concentrations and corresponding volumes used for the tests.

The oil cloud homogeneity is difficult to ascertain, however the dispersion time, from 2 to 8 seconds (usually 4 to 6) was considered sufficient to get a homogeneous cloud.

3 CFD modelling of explosions

FLACS is a CFD tool developed for simulating gas explosions. For risk assessment purposes, gaseous fuels are used to represent aerosols in the current version of the software. Specifically, for transformer studies, oil mists are represented using the butane equivalent fraction, determined according to molecular weight and heat of combustion of the gaseous species, and fuel concentrations. As the current study demonstrates, the simplified solution provides reasonable estimates. However, there is significant potential for improving the models for multiphase flows and combustion. The model for gas explosion used in FLACS is then quickly exposed.

FLACS solves conservation equations for mass, momentum, enthalpy mixture fraction and the turbulent parameters k and ε. Models for simulating turbulent reactive flows in complex geometries, such as offshore modules, have been analysed and presented by Arntzen [12]. The most important aspects that determine the course of a gas explosion in a complex geometry are the production of turbulence and the corresponding increase in the combustion rate during the explosion. In FLACS, the turbulent flow field is modelled with the k-ε turbulence model. Sub-grid models are used for describing production of turbulence from the part of geometry that is not fully resolved on the grid. Turbulent combustion is modelled with a burning velocity model and a flame model which incorporates the volumetric rate of combustion. In the so-called β flame model, the reaction zone is resolved with about 3 grid cells and requires correction models for small flame radii and burning towards walls where the reaction zone is thinner. The initial phase of flame propagation is described by a model that accounts for the effects of flame instabilities by introducing a quasi-laminar burning velocity that varies as function of flame radius and the laminar burning velocity. As the flow field becomes turbulent, the flame uses a turbulent burning velocity S_T based on experimental data collected by Abdel-Gayed et al [13] and summarized in a correlation by Bray [14].

Models for describing dispersion of droplets have been implemented in FLACS but there is no dedicated combustion model for aerosol explosions. One of the challenges associated with aerosol combustion is the different combustion regimes: homogeneous combustion, heterogeneous combustion and the transition region where both homogeneous combustion and heterogeneous combustion take place at the same time [15]. Homogeneous combustion dominates when the flammable cloud consists of small droplets, typically (less than 10 μm diameter); the droplets vaporize and mix with the air before the flame front reach them, resulting in a reaction zone that resembles a premixed flame. Larger droplets (greater than about 30μm) are typically partially evaporated by the time the flame front reaches them. The mixing is not complete which leads to a regime with individual droplet burning. In the transition region, both phenomena occur simultaneously. This regime may be the most dangerous since the particles can be big enough to wrinkle the flame and small enough to evaporate rapidly, and hence accelerating the flame. The long-term goal is to develop a specific burning velocity and flame models for FLACS to allow simulation of mist explosions. Existing models are currently under investigation for possible implementation. Bowen [15] reviewed different theories including the work by Ballal and Lefebvre [16], Polymeropoulos [17] and Aggarwal [18-20].

4 Results and discussion

The LICOREFLA experiments were simulated with FLACS. Initially, two grid resolutions were used to explore grid dependency issues, but 2cm and 5cm cells resulted in similar results. The grid of 5cm was chosen for the rest of the simulations. Figures 2 to 4 summarize the results for hexane, decane and three classes of oil (1, 2 and 3).

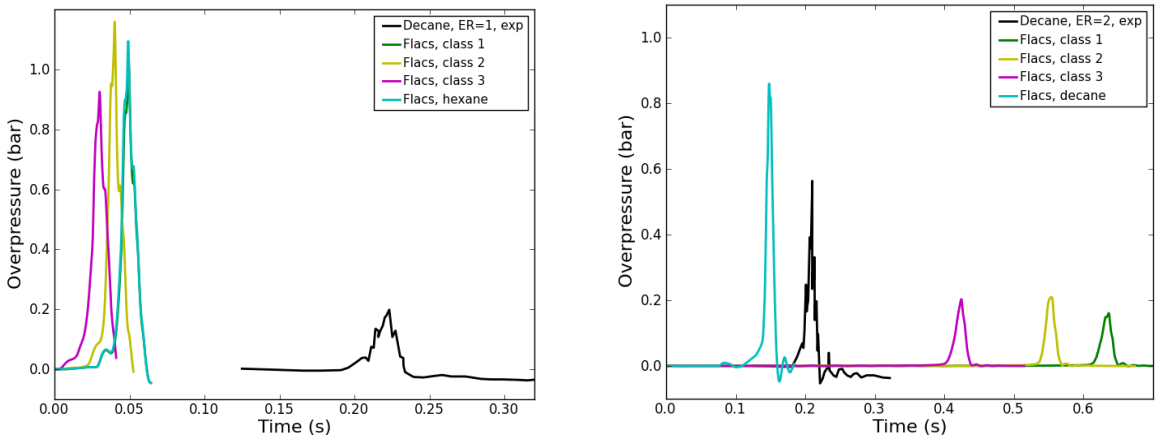

Figure 2: Overpressure as a function of time for the geometry with two baffles. On the left, decane with ER=1. On the right, decane with ER=2. The black graphs represent experimental results.

The blue line corresponds to numerical results assuming complete evaporation of decane. The oil classes 1, 2 and 3 represent different fractions of oil in the cloud; or different fractions of butane in the simulations. They differ in terms of the amount of added oil mist having combustion energy equal to *n* times the amount of gas from cracked oil (this methodology was developed in relation to transformer explosions).
For the decane with ER=1, FLACS overpredicts the overpressure for both methods used. With ER=2, assuming complete evaporation of decane leads to over-prediction while the butane equivalent results in under-prediction.

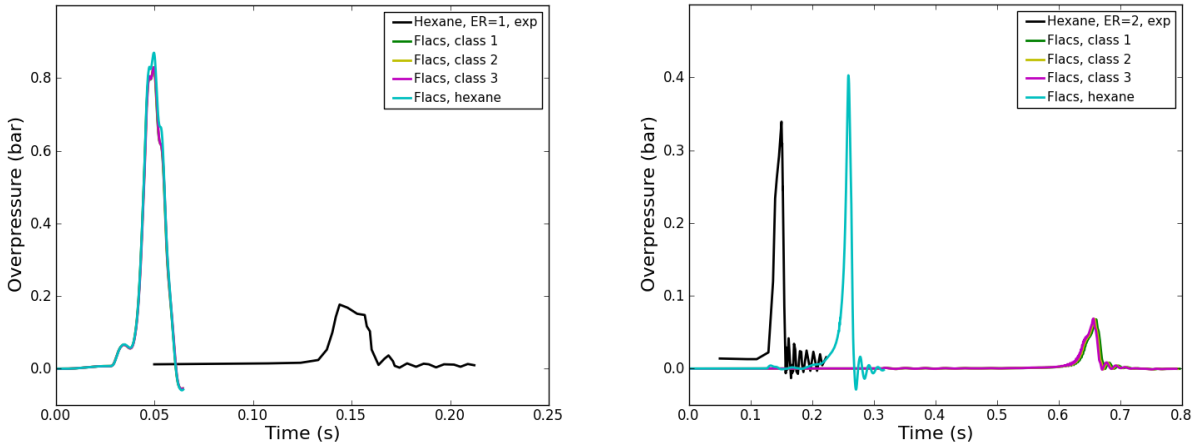

Figure 3: Overpressure as a function of time for the geometry with one baffle. On the left, hexane with ER=1. On the right, hexane with ER=2.

The results in Figure 3 are similar to those for decane, the model with all the hexane as a gas is overpredicting for ER=1 and 2, while the butane equivalent overestimates for ER=1 and underestimates for ER=2.

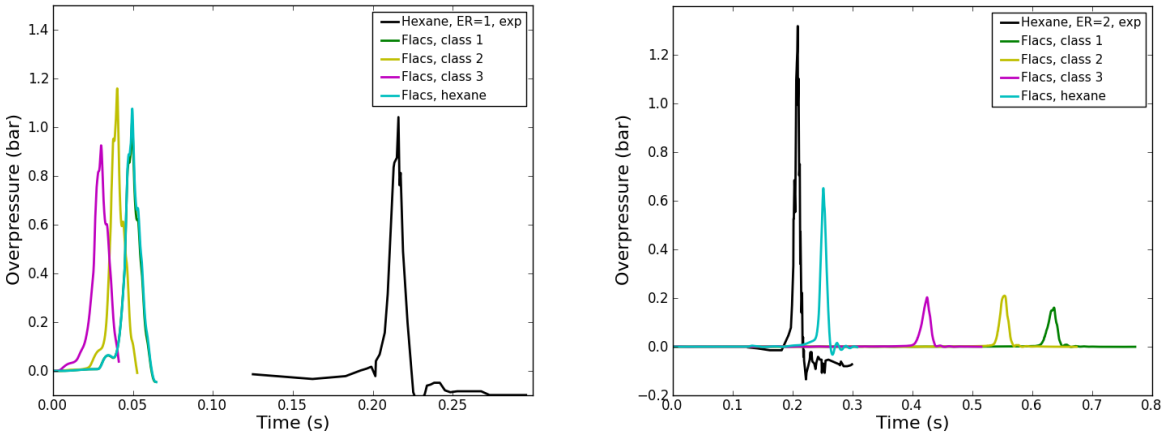

Figure 4: Overpressure as a function of time for the geometry with two baffles. On the left, hexane with ER=1. On the right, hexane with ER=2.

In Figure 4, the overpressure obtained for an equivalent ratio of 1 was similar in the experiment and simulations. However, the pressure peak is arriving too soon in the simulation. The previous results apply for ER=2, FLACS underestimates the peak pressure.

Hexane and decane experiments give greater overpressures at ER=2 compared to ER=1. This can be explained in terms of the loss of oil inside the rig. The loss due to walls or fall-out is so that at ER=1 we lose approximately half of the liquid and obtain a lean mixture, then for ER=2 we obtain an actual ER of 1 inside the rig.

5 Conclusion

In this study, for both experiments at ER=1, lean mixture in the rig, it seems that a cloud where all the droplets have evaporated is more dangerous than a cloud with droplets in the transition zone. However for ER=2, which would correspond to a close to stoichiometry mixture in the rig, it seems that a cloud of gas and droplets (experiments) could lead to pressure higher than the equivalent cloud with only gas (simulations), which tends to confirms that mist explosions cam lead to greater risks than gas explosions.

FLACS performs relatively poorly for the aerosol explosions investigated in this study and further development is required to simulate such phenomena properly. However, some data such as the turbulence intensity in the cloud could not be measured and this complicates the validation work. There is a definite need for experimental data of high quality, and the validation study should be extended to experiments performed at larger scales.

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