VALIDATION OF CFD CALCULATIONS AGAINST IGNITED IMPINGING JET EXPERIMENTS

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ABSTRACT

Computational Fluid Dynamics (CFD) tools have been increasingly employed for carrying out quantitative risk assessment (QRA) calculations in the process industry. However, these tools must be validated against representative experimental data in order to have a real predictive capability. As any typical accident scenario is quite complex, it is important that the CFD tool is able to predict combined release and ignition scenarios reasonably well. However, this kind of validation is not performed frequently, primarily due to absence of good quality data. For that reason, the recent experiments performed by FZK under the HySafe internal project InsHyde (http://www.hysafe.org) are important. These involved vertically upwards hydrogen releases with different release rates and velocities impinging on a plate in two different geometrical configurations. The dispersed cloud was subsequently ignited and pressures recorded. These experiments are important not only for corroborating the underlying physics of any large-scale safety study, but also for validating the important assumptions used in QRA.

Blind CFD simulations of the release and ignition scenarios were carried out prior to the experiments to predict the results (and possibly assist in planning) of the experiments. The simulated dispersion results are found to correlate reasonably well with experimental data in terms of the gas concentrations. The overpressures subsequent to ignition obtained in the blind predictions could not be compared directly with the experiments as the ignition points were somewhat different, but the pressure levels were found to be similar. Simulations carried out after the experiments with the same ignition position as those in the experiments compared reasonably well with the measurements in terms of the pressure level. This agreement points to the ability of the CFD tool FLACS to model such complex scenarios well. Nevertheless, the experimental set-up can be considered to be small-scale and less severe than many accidents and real-life situations. Future large-scale data of this type will be valuable to confirm ability to predict large-scale accident scenarios.

1. INTRODUCTION

Computational Fluid Dynamics (CFD) calculations have been used more and more to perform quantitative risk assessments in recent years, especially in the oil and gas industry. Based on predicted consequences of a range of potential accident scenarios a risk level is estimated. However, we need to be careful before applying a CFD tool to carry out such risk assessments. The tool needs to be well validated against a range of relevant experiments (with studies on variations of various important parameters that may affect explosion loads and hence risk). Nonetheless, when CFD consequence prediction tools are validated, there is a significant focus on basic situations, like free jet releases for dispersion, or pre-mixed homogeneous gas mixtures for explosions. It must be pointed out that the typical accident scenario is usually more complicated, possibly involving time varying releases impinging on equipment, with delayed ignition of a non-homogenous and possibly turbulent mixture. When aiming for increased precision in risk assessment methods there is a need to validate consequence tools for this added complexity. For post-accident simulations, it is obvious that there is a

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need to reproduce the complex physics of the accident scenario, and validation of tools for the combined release and ignition scenarios is important. For the modelling of such a situation, validation or verification against idealized scenarios is far from sufficient. A very important cause of this gap in "real" validation of CFD tools is that it is challenging to perform good experiments with such a complexity. Good experimental data involving scenarios reminiscent of those seen in real situations are few and far between, especially at large scales.

Over the past few years, the focus on carrying out safety studies for hydrogen applications has increased, and the use of CFD has increased. However, the CFD tool needs to be well validated against relevant experiments. With these considerations, a strong effort has been made in the past few years to learn more about hydrogen explosions and improve FLACS in that area. We have carried out dedicated research projects involving varied small-scale experiments, combined with simulations and model improvements in order to improve the validation database for hydrogen safety predictions [1]. Simulations of many large-scale experiments from various external sources have also been carried out. This includes explosion simulations for Sandia FLAME facility [1], Fh-ICT 20 m hemispherical balloon [2], SRI confined tube [3], Fh-ICT lane experiments [4], McGill Detonation Tubes [5], and more. Dispersion simulations have been carried out to validate predictive capabilities for sonic jets [6] (e.g. HSL tests, INERIS experiments, and FZK tests) and subsonic jets (INERIS garage experiments [7], Swain experiments [6], GexCon low momentum release experiments [8]). Other studies have also been carried out, but are not available presently in open literature [9]. Studies presented in References [2], [7] and [8] have been carried out as a part of the benchmarking activities in the HySafe project.

However, none of the experiments used for validation involved simultaneous dispersion and ignition. For this reason, recent experiments carried out by FZK as a part of HySafe internal project InsHyde are significant. This study involved vertically upwards hydrogen releases impinging on a horizontal plate or hood (plate with side walls). After a time delay, the dispersed cloud was ignited and pressures recorded. In the weeks prior to the planned experiments, we performed several blind CFD simulations to predict the outcome of the proposed experiments, and if possible, to help the planning. After the experiments were reported, the quality of the blind predictions was evaluated. The gas concentrations of the impinging jets were generally well predicted, both along and across the jet. The explosion experiments were performed with a slightly different ignition position than the blind predictions, but still the predicted pressure level was representative of the observations. Simulations with the exact ignition positions of the experiments were performed after the tests, and confirmed the ability of the CFD tool FLACS to predict the pressures from ignition of non-homogeneous hydrogen clouds. This type of experiments provides a possibility to validate important assumptions used in probabilistic quantitative risk assessments, which are necessary to limit number of scenarios studied (e.g. equivalent stoichiometric cloud size methods). Such calculations are performed and are presented in the following sections.

2. BRIEF DESCRIPTION OF EXPERIMENTS

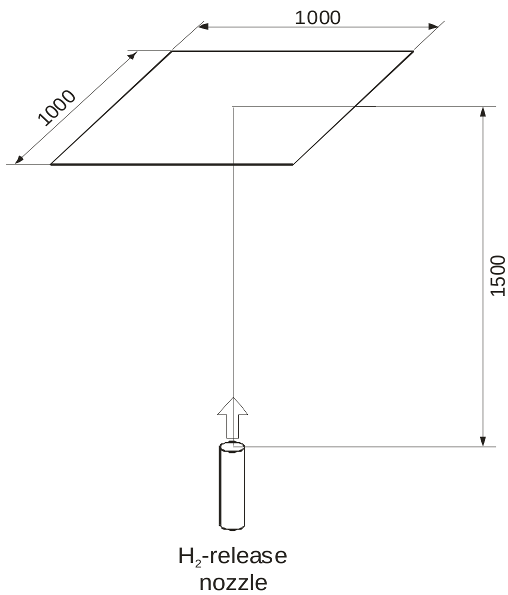
Nine hydrogen release scenarios were investigated in the experiments, covering three different diameters of the circular release nozzle (100 mm, 21 mm, and 4 mm) with three different constant hydrogen release rates each. These scenarios are summarized in Table 1, along with the corresponding exit velocities and the total release time. It should be pointed out that the total hydrogen inventory was fixed at 10 g in all cases. Two different geometrical configurations were considered in the experiments:

1. Square horizontal plate (dimension 1.0 m) at a distance of 1.50 m above the release nozzle.
2. Same set-up as configuration 1 but with four additional vertical sidewalls of 0.50 m height, forming a downward open hood with a volume of 500 litres above the release nozzle.

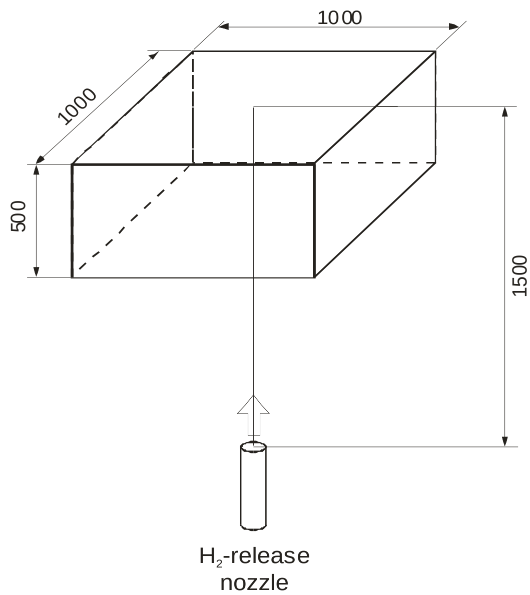
A schematic view of the two configurations is presented in Figure 1. Hydrogen concentrations between the nozzle and plate were determined by collecting gas samples in eight cylinders. Since a stable plume needs some time to establish above the release, measurements were performed at times close to the end of the duration of the hydrogen release. The hydrogen content of the sample taking cylinders was determined using a gas analysis system (Fisher-Rosemount, Series MLT) with a measuring range from 0 to 100 vol. % H_2 and 0 to 100 vol. % O_2. The concentration measurements were also used to determine appropriate positions for the ignition source in the subsequent combustion experiments.

Table 1. Release scenarios investigated in the experiments

Experimental series	Nozzle-diameter [mm]	Exit velocity [m/s]	Mass flow [g/s]	Release duration for 10 g H_2 inventory [s]
A	100	0.2	0.14	71.3
B	100	1	0.7	14.3
C	100	5	3.5	2.85
D	21	5	0.15	64.7
E	21	100	3	3.23
F	21	200	6	1.62
G	4	100	0.14	70
H	4	200	0.29	35
I	4	400	0.57	17.5



Configuration 1 (Horizontal plate)



Configuration 2 (Horizontal plate with sidewalls)

Figure 1. Configurations investigated in the experiments

The released hydrogen was ignited using a high frequency spark at two different ignition positions (0.8 and 1.2 m above the release nozzle). Combustion overpressure measurements were performed using ten piezoelectric pressure gauges (PCB, Models 112A21, 113A21 and 113A31). Eight of these sensors were fixed to a bar in a distance of twenty centimetres to each other. The two remaining pressure transducers were installed to the same bar at locations in between these positions. The whole bar was then installed either horizontally or vertically at a certain height and distance to the axis of the hydrogen release. Metallic grid net layers in various different configurations were used in the experiments in order to accelerate the flame and seek to obtain “worst-case” results. However, since their description was not available prior to the simulations, they were not considered and hence will not be described in this article. More details of the experiments can be found in Reference [10].

3. SIMULATION DETAILS

All the simulations have been carried out using the CFD tool FLACS. FLACS is a computational fluid dynamics (CFD) tool that solves the compressible Navier-Stokes equations on a 3-D Cartesian grid. The basic equations used in the FLACS model as well as the explosion experiments to develop and validate FLACS initially have been published [11,12]. Second order schemes (Kappa schemes with weighting between 2nd order upwind and 2nd order central difference, delimiters for some equations) are used to solve the conservation equations for mass, impulse, enthalpy, turbulence and species/combustion. A distributed porosity concept is applied. FLACS can therefore be used to simulate most kinds of complicated geometries using a Cartesian grid. Large objects and walls are represented on-grid, and smaller objects are represented sub-grid. Sub-grid objects will contribute with flow resistance, turbulence generation and flame folding (explosions) in the simulation. A good description of geometry and the coupling of geometry to the flow, turbulence, and flame is one of the key elements in the modelling. In FLACS a "beta" flame model is applied in which the reaction zone becomes 3-5 grid cells thick. The burning velocity is primarily controlled by diffusion of reaction products. A flame library decides the laminar burning velocity as function of gas mixture, concentration with air, pressure, temperature, oxygen concentration in air and more. Initial "quasi-laminar" flame wrinkling will increase the burning velocity with distance. With increasing turbulence a turbulent burning velocity replaces the quasi-laminar. The real flame area is described properly and corrected for curvature at scales equal to and smaller than the reaction zone. All flame wrinkling at scales less than the grid size is represented by sub-grid models. FLACS uses a standard k-ε model for turbulence. However, some modifications are implemented, the most important being a model for generation of turbulence behind sub-grid objects and turbulent wall functions [13].

The experimental geometry for the two different configurations as represented in FLACS is presented in Figure 2. The computational grid used in the simulations for the dispersion calculations is shown in Figure 3 for the case of a single plate for the 100 mm nozzle. Please note that similar grid resolution is used for the other geometries and scenarios with the same nozzle size. The grid was made coarser away from the orifice and the enclosing plates in order to improve computational efficiency. However, the grid was appropriately adjusted for the smaller nozzles, as finer grid resolution is required in the vicinity of the orifice to model the leaks properly. The summary of the grid sizes is also presented below in Figure 3.

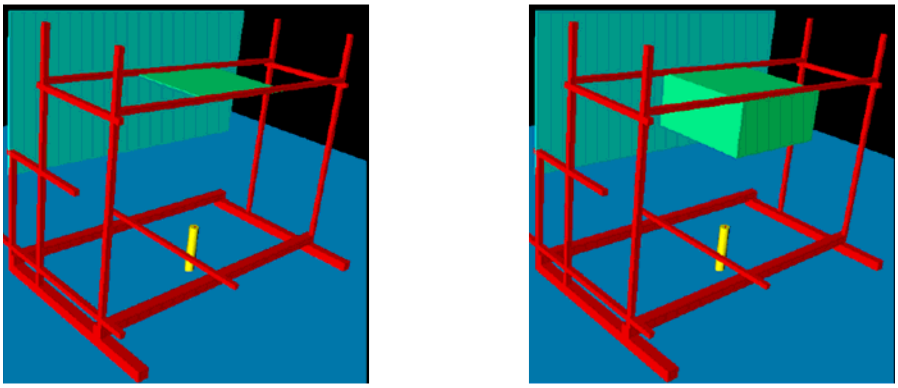
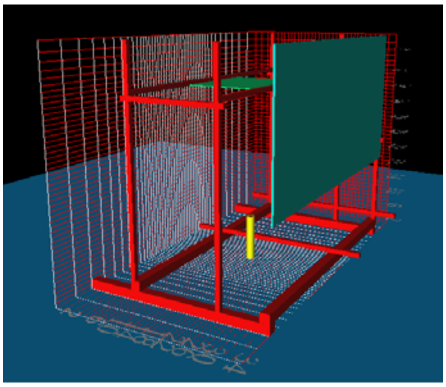


Figure 2. Representation of the two experimental configurations in FLACS

Simulation time on single CPUs vary from a couple of hours to a few days, depending on nozzle size, leak velocity and duration of leak. The release scenarios with a small nozzle and long release time are the most time consuming. The simulations were carried out in quiescent conditions with passive boundary conditions (no wind). For combustion simulations with real gas cloud, the dispersion results were dumped and the simulations were restarted with the appropriate explosion grid (equidistant in all directions) following the grid guidelines of the CFD program. The explosion calculations are performed on a finer grid with 2.5 cm grid resolution in the interesting region. The refinement was necessary to comply with the grid guidelines for explosions, which require a certain minimum number of grid cells across a gas cloud.



Nozzle size	Normal grid resolution in interesting region	Grid resolution near the leak	Total grid cells
100 mm	5 cm	5 cm	70,312
21 mm	5 cm	2 cm	89,817
4 mm	5 cm	0.5 cm	135,877
Explosion	2.5 cm	N.A.	251,720

Figure 3. A sketch of the computational grid used for the dispersion simulations for the 100 mm nozzle along with a summary of the grid resolution for all dispersion and explosion calculations

4. RESULTS AND DISCUSSION

This section presents selected results obtained during the experiments and comparisons with relevant simulation results. The results obtained in the dispersion study are presented first and the pressure loads subsequent to ignition of dispersed clouds are presented next. Detailed results of all the simulations that were performed, compared with experiments are available in Reference [14].

4.1 Dispersion

In Figure 4, concentration profiles from FLACS blind predictions for all three release rates for the 100 mm and 21 mm nozzles for the plate geometry are compared with experimental results. Please note that the release nozzle is located at a height of 0.5 m. A detailed comparison of simulated versus reported profiles from experiments indicates that there is a reasonable correlation between predictions and experiments for the tests with 100 mm nozzle but some deviation can still be seen. In general, the simulation results for releases from the largest nozzle show an underprediction near the release nozzle, and an overprediction away from the release nozzle. The three 21 mm nozzle release experiments seem to be predicted with good precision for all three release rates.

The results with 4 mm nozzle for the same geometry (not shown) indicate some deviation between simulations and experiments as FLACS underpredicts the concentrations somewhat, e.g. at a position of 0.2 m above the jet, a concentration of 16% H_2 is predicted with FLACS whereas observed concentrations are in the range 21-25%. One reason for this deviation could be that it was expected that for this nozzle size, the resulting flammable plume would not be interesting from a risk point of view. As small releases may lead to quite long simulation times, we did not follow the grid embedding guidelines strictly. The somewhat larger grid cell around the leak than recommended leads to a small overestimation of the dilution in the plume, and hence results in a lower concentration. As the resulting gas cloud sizes were indeed found to be insignificant, these simulations were not rerun with a better grid.

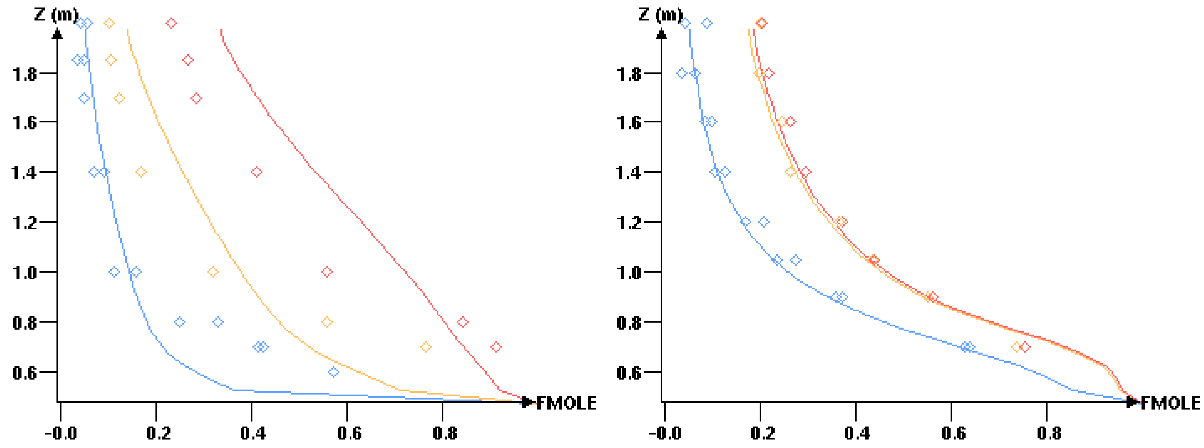


Figure 4. Comparison of experimental concentration profiles (top) and FLACS predicted concentration contours (bottom) for releases from 100 mm (left figures) and 21 mm (right figures) nozzle (plate geometry).

In Figure 5, the lateral distribution of concentration is shown for the experiments with release from the 100 mm and 21 mm nozzle and compared to blind predictions. For the 100 mm nozzle (left figures), it was found that the concentration from the lowest release rate was somewhat underestimated. However, this may be a result of the grid resolution applied. Since the plume width is only 10-15 cm, and the grid resolution is 5 cm (no control volume in the middle of the release), the deviation can be easily understood. For the intermediate leak rate (0.7 g/s) a much better correlation is seen, for the large leak rate the plume width is well predicted, but some underprediction of concentration is observed. For the 21 mm nozzle (right figures), it can be seen that the simulated lateral concentrations correspond well with the experimental recordings for all three release rates. Both the maximum concentration and plume width are predicted with good accuracy. In Figure 6, a BOS (Background oriented Schlieren) picture with numerical measurements added (21 mm nozzle, 3 g/s) is shown and compared to a predicted concentration profile. The measured concentrations and shape of plume correspond well to the predictions.

Next, we consider the second geometrical configuration. Concentrations obtained in the experiments from releases from the two large nozzle sizes in the hood geometry are presented in Figure 7. For the 3.5 g/s release (100 mm nozzle), the lateral distribution of concentration from FLACS predictions corresponds well with experimental data both for 1.25m and 1.05m elevations (see bottom part of Figure 7). However, the experimental jet axis concentration is 23% whereas a value of more than 30% is predicted by FLACS. Also the results for the 0.7 g/s release compare quite well with experiment, while the concentrations resulting from the 0.14 g/s release may be slightly underpredicted. In the simulations, the grid resolution was 5cm, i.e. the slowest leak was resolved by a region 2×2 grid cells across. A result of this is that there is no grid cell exactly on the central axis of the jet. It is likely that a higher resolution of the leak could make the predictions even better. One should also take into account that the experimental recordings have many uncertainties, as average concentrations will be approximated over a certain volume. This may also lead to deviations between predictions and observations in some cases. The comparison of lateral concentrations resulting from releases from the 21 mm nozzle into the hood shows good correlation for the 3 g/s release, whereas the concentrations for the 0.15 g/s release may be somewhat too low in simulations. It is a question whether a better grid resolution across the jet will be required for such low momentum releases. The results may also be influenced by the time the results are extracted. For the 3 g/s release, a steady state may be reached (due to the high momentum), whereas for the 0.15 g/s the concentrations in the hood will increase throughout the duration of the leak. In Figure 8, the experimental BOS picture with numerical measurements added (21 mm nozzle, 3 g/s) for the hood geometry is shown and compared to a predicted concentration profile. The measured concentrations and shape of plume correspond well to the predictions.

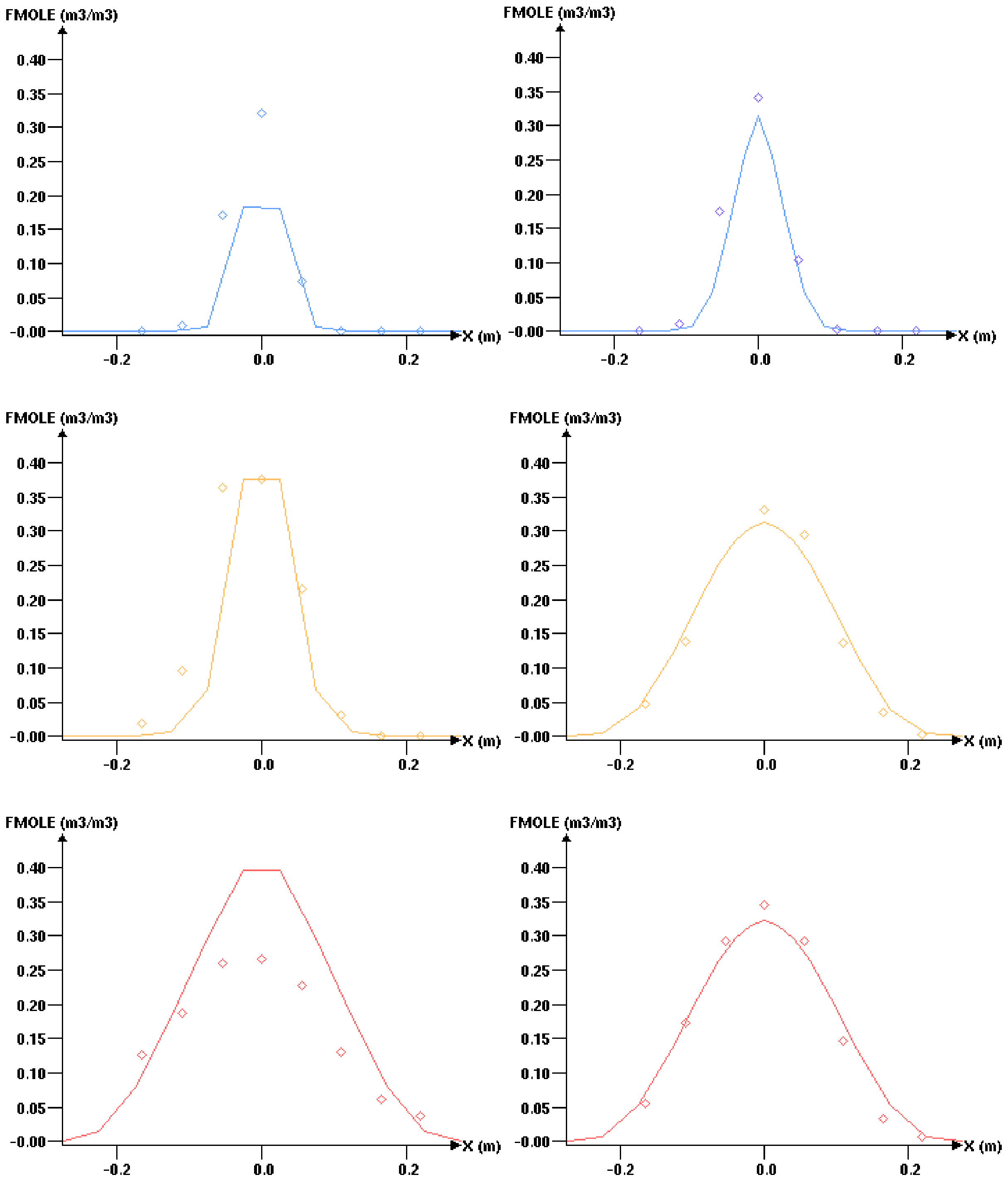


Figure 5. Experimental recorded horizontal concentration distribution at the elevation chosen for ignition versus FLACS predicted horizontal concentrations for release from 100 mm nozzle: 0.14 g/s (upper left), 0.7 g/s (middle left) and 3.5 g/s (lower left) and for 21 mm nozzle: 0.15 g/s (upper right), 3.0 g/s (middle right) and 6.0 g/s (lower right).

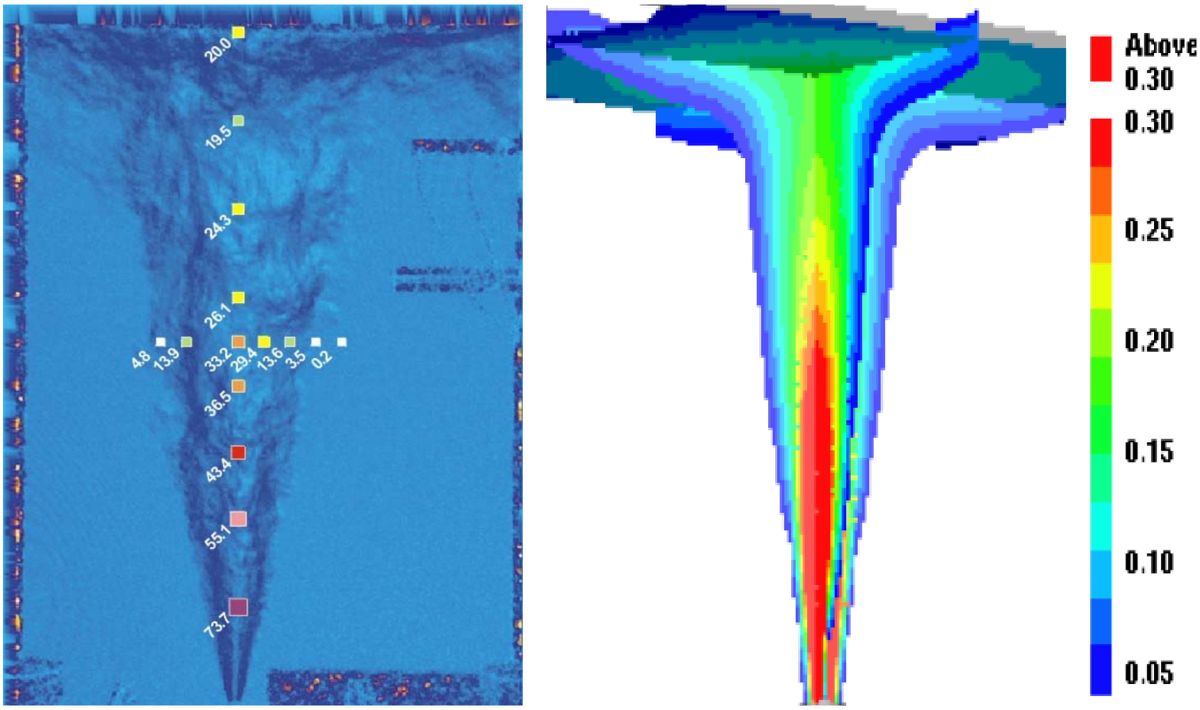


Figure 6. Comparison of experimental photograph/recording with FLACS predicted plume shape and concentrations for release from 21 mm nozzle (3 g/s) towards plate.

4.2 Explosion

This section correlates experimental data and simulation predictions for overpressures obtained subsequent to ignition of dispersed clouds. We performed a number of explosion simulations in which the realistic gas clouds were ignited during the release. The results of the dispersion simulations were dumped at various times and the simulations were restarted using a uniform grid that is required for carrying out explosion calculations. In Figure 9 pressure curves for the simulation giving the highest pressures among all the situations are presented. It can be seen that the maximum pressure of about 80 mbar is seen. It must be noted that several of the explosion cases cannot be directly compared to the predictions performed with FLACS as experiments used flame accelerating obstacles whose dimensions can not easily be described in detail. Further, for the experiments where these obstacles were not used, the ignition points in the simulations were somewhat different from those in the experiments. Still the pressure levels are comparable to those reported blind.

For analyzing the danger of ignition of dispersed cloud, a concept called the equivalent stoichiometric gas cloud has been developed through our work towards quantitative risk assessment (QRA) for oil and gas applications. Herein, the dispersed gas clouds with non-homogenous distribution of gas and turbulence from jet are normally replaced by smaller equivalent stoichiometric gas clouds, *Q*9 [15]. *Q*9 cloud is a scaling of the non-homogeneous gas cloud to a smaller stoichiometric gas cloud that is expected to give similar explosion loads as the original cloud (provided conservative shape and position of cloud, and conservative ignition point). It is defined as $Q9 = \sum V \times \mathrm{BV} \times E \,/\, (\mathrm{BV} \times E)_{\mathrm{stoich}}$. Here, V is the flammable volume, BV is the laminar burning velocity (corrected for flame wrinkling/Lewis number effects), E is volume expansion caused by burning at constant pressure in air, and the summation is over all control volumes. As a practical guideline, it is recommended to choose the shape of the cloud that will give maximum travel distance from ignition to end of cloud for smaller clouds. For larger clouds, end ignition scenarios with longer flame travel should also be investigated. This concept is useful for QRA studies with many simulations, and has been found to work reasonably well for safety studies involving natural gas releases [15].

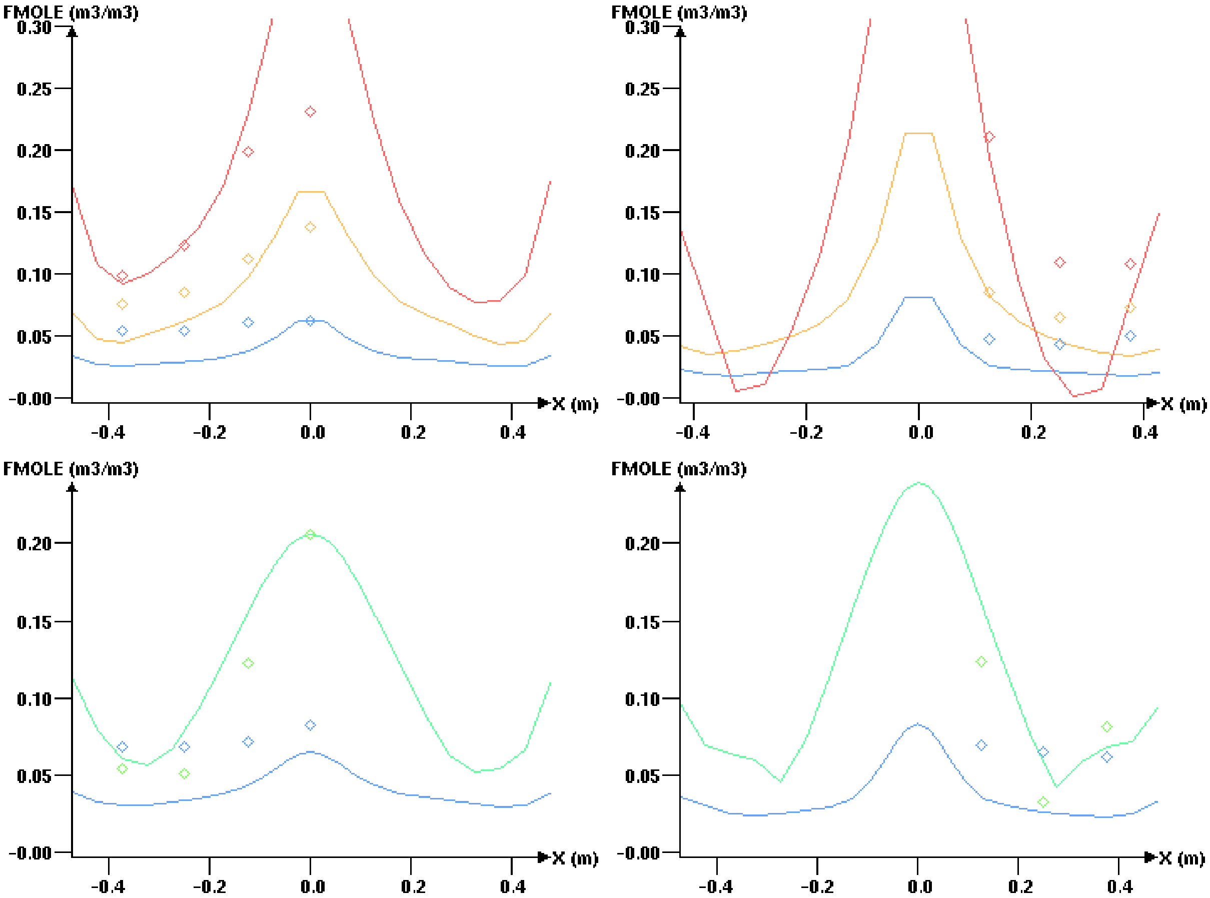


Figure 7. Comparison of experimental recordings with FLACS predicted concentrations in the hood geometry for 100 mm nozzle (upper figures) and 21 mm nozzle (lower figures) for measurement location 1.25m above leak (left figures) and 1.05m above leak (right figures). Simulated release rates of 0.14 g/s (blue), 0.7 g/s (orange) and 3.5 g/s (red) for 100 mm nozzle and 0.15 g/s (blue) and 3 g/s (green) for 21 mm nozzle are shown.

As one of the goals of this study is to develop corresponding risk assessment methods for hydrogen systems, we have investigated the applicability of this concept to the present system. The size of the equivalent stoichiometric gas cloud as a function of time for the two scenarios shown in Figure 6 and 8 is presented in the left plot of Figure 10, where it can be seen that the hood geometry presents a greater risk as expected. In the right plot in Figure 10, the experimental pressures predicted by simulations for all different scenarios (plate and hood geometry) are summarized as a function of an "equivalent" stoichiometric gas cloud size *Q*9. This figure only includes blind simulations carried out prior to the experiments for two different ignition positions: center and edge. For the plate only geometry it can be seen that the maximum pressure is 40 mbar; however, the majority of predicted explosion pressures are in the range 0-20 mbar. Further, it must be pointed out that even if a pressure of 40 mbar was reported in the worst-case, the highest pressure was due to a short local initial pressure transient in connection to ignition, and the main pressure level is rather 20 mbar than 40 mbar. The lines indicate reference calculations using homogeneous stoichiometric gas clouds. In this plot, the red line indicates the pressure level found in quiescent explosion scenarios with a conservative cloud location and ignition point (rectangular stoichiometric cloud located centrally towards the plate with ignition centrally on plate, but turbulence from jet ignored) for the hood geometry while the blue line indicates the corresponding pressure level for the plate geometry.

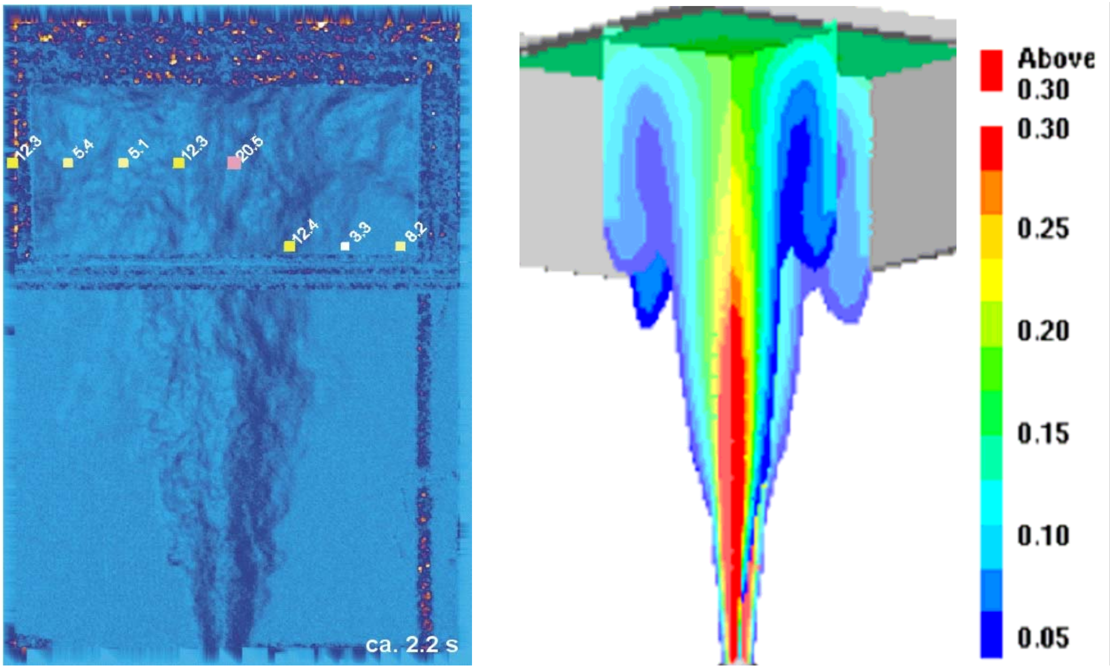


Figure 8. Comparison of experimental photograph/recording with FLACS predicted plume shape and concentrations for release from 21 mm nozzle (3 g/s) in the hood geometry.

The plot shown in Figure 10 indicates that the ignition of such smaller idealized stoichiometric clouds is a good approach to indicate the expected overpressure level. For the plate situation, the "blue" line corresponds well with the simulated realistic pressures. However, for the hood situation one of the simulated explosions gives 30% higher pressure than the red curve, but still the "red" curve gives a representative pressure level for the situation with the hood. These higher pressures could be explained by the fact that jet-induced turbulence is ignored while reference pressures are calculated. As can be seen for the experimental pressures in Figure 11, this pressure level is generally representative for what was observed in the experiments. In the hood geometry, the maximum predicted pressure level reached 80 mbar, but most of the explosions produced pressures in the range 20-40 mbar (some were below 10 mbar). In some cases, the overpressures obtained are higher than those predicted by explosion simulation of stoichiometric scenarios. This can be explained by the fact that jet-induced turbulence is neglected while reference results using equivalent stoichiometric clouds are obtained. In some cases, jet-induced turbulence can cause the overpressures to go up by a factor of 2-3.

Due to a different ignition point used in the experiments compared to the initial simulations, we resimulated 8 explosion tests again in order to be able to compare with experiments directly. Also, there may be a small difference in time of the ignition between simulations and experiments. This should not be important for the plate scenarios, but it could be important for low momentum cases in the hood configuration as gas may continue to accumulate with longer release time. In Figure 11 it can be seen that 3 of the FLACS simulations give explosion pressures in the hood of 10-30 mbar for ignition position 1.2m above release location, which corresponds well to the measured pressures of 5 to 20 mbar. The bottom part of Figure 11 presents a similar plot for some ignited scenarios with ignition at 0.8m above jet. Please note that all these simulations have been performed for realistic gas clouds obtained as a result of the hydrogen release. Here it should be taken into account that the pressure reported by FLACS simulations also includes very narrow oscillations that may be filtered out in the experimental interpretation. For one of the cases (100 mm nozzle, hood geometry) for the higher ignition position, FLACS predicts a much higher pressure (60 mbar) than is seen in experiment (10 mbar). One possible explanation to this could be that the FLACS simulation is ignited at a later time than the experiment, and thus that the gas accumulation inside the hood may be significantly different. No details of this are available at the present time. From the FLACS simulations for the lower ignition location, it can be seen that there is a local (short duration) pressure transient around ignition (0.8m) that is not seen (or reported) in the experiments. Inside the hood simulated pressures range from 10-20 mbar, and 50 mbar for one case (21 mm hood, 6 g/s). For all four cases, the FLACS pressures correspond reasonably well with the observations.

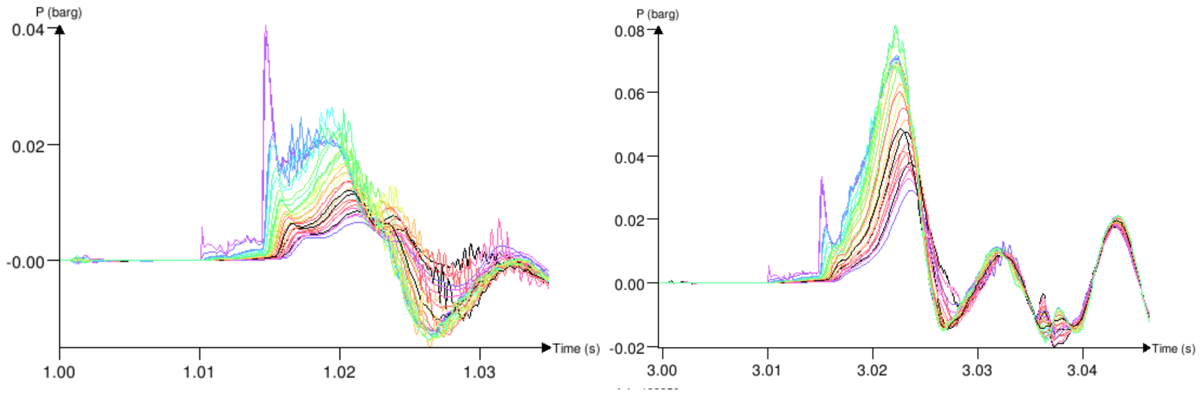


Figure 9. Worst-case explosion pressures resulting from exploding non-homogenous clouds from dispersion simulations: (Left) Plate Geometry and (Right) Hood Geometry

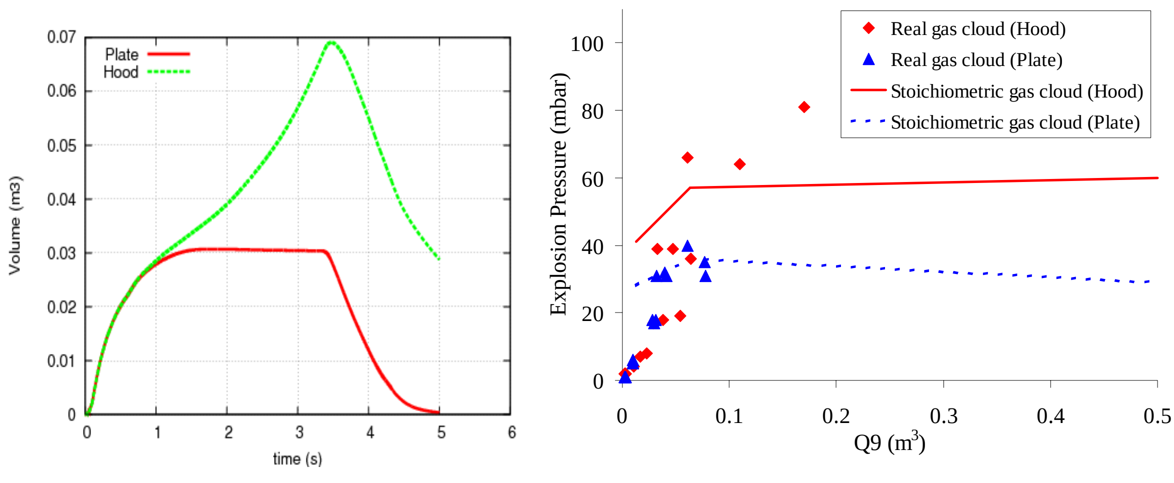


Figure 10. (Left) Equivalent Stoichiometric gas cloud as a function of time for the 21mm release scenarios (3 g/s) for the plate and hood geometries (see Figures 6 and 8). (Right) Blind predicted overpressures in hood (red) and plate (blue) configurations as function of estimated Q9 equivalent cloud size (FLACS QRA-method) for ignited leaks. Reference calculations with homogenous stoichiometric gas clouds are included.

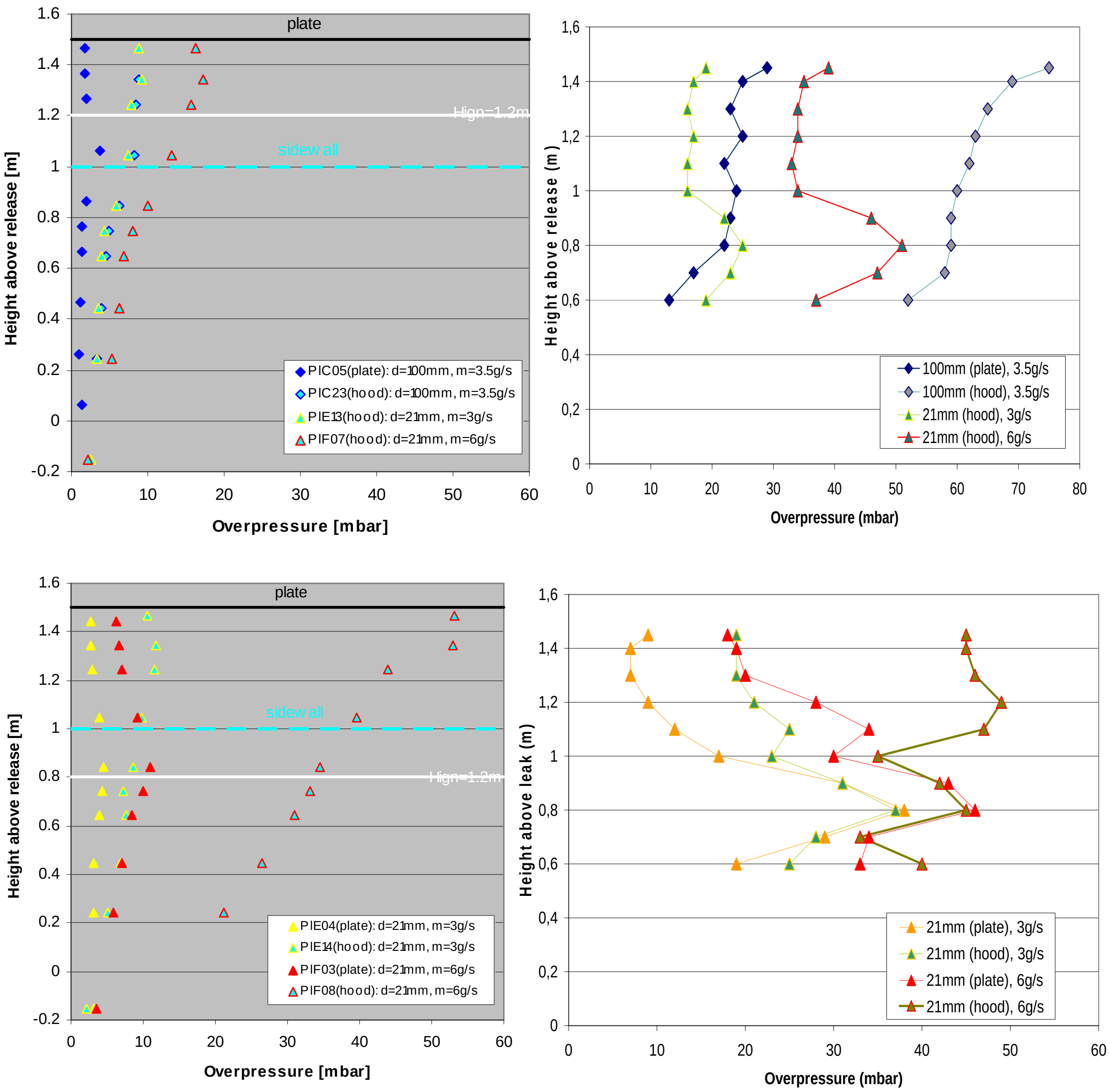


Figure 11. FZK experimental pressures (left) compared with FLACS explosion pressures (right) of ignited jets for ignition location along the jet axis 1.2m from release nozzle (top pictures) and 0.8 m from release nozzle (bottom pictures). With FLACS only pressures from position 0.6m and up were reported.

The results of the comparison of explosion pressures between experiments and simulations are encouraging. It can be concluded that simulated explosion pressures when igniting releases correspond well to the experimental observations. This points to the ability of FLACS to model the combined phenomenon of dispersion and direct ignition of non-homogeneous clouds with jet induced turbulence. A further important observation is that our risk assessment approach, in which the reactivity of the dispersed cloud is translated into an equivalent stoichiometric smaller cloud size (without initial turbulence, but with conservative cloud position and shape, and ignition location), gives a good indication of expected overpressures.

5. CONCLUSIONS

A significant number of CFD simulations were performed with FLACS as blind predictions of experiments that were performed by FZK. Based on the comparison between observations and predictions, the following conclusions can be made:

1. In general leak scenarios were well predicted. The best predictions were seen for the high momentum releases (21 mm nozzle) while somewhat lower precision was seen for 4 mm releases (which were not modeled too accurately as the leaks were too small for dangerous gas clouds to be generated) and also for the low momentum release scenarios with 100 mm nozzle. With a more accurate source modeling (better resolution of leak) for the 4 mm releases, as well as finer grid cells for the 100 mm releases with very low momentum, even better results could be expected. One should also keep in mind that the calculations were performed in a typical risk assessment project setting, in which many CFD calculations were simulated quickly (within 1-2 weeks). With more focus on accuracy of single scenarios, a better grid resolution would have been applied for the 4 mm leaks and possibly the 100 mm leaks with low momentum.

2. The initially modeled explosion scenarios deviated from the experiments with regards to ignition position, and no direct comparisons could therefore be performed. Still the predicted pressure levels with FLACS were similar to what was observed in the experiments, both for ignition of non-homogeneous clouds during releases, but equally importantly, the explosion pressures from the estimated equivalent gas clouds (Q9-method) also corresponded well with the observations in the experiments. After the experiments some ignition cases were resimulated with the same ignition locations that were used in the experiment, and for 7 out of 8 examples the simulated overpressures corresponded well to the experimental observations. The case with significant deviation may be due to different ignition times.

The work performed in this article is very important to build confidence in the use of CFD tools for modeling combined release and ignition scenarios. In general, satisfactory results are seen. It is very important for model developers to have access to good quality data. However, only limited tests data of this type is available and as a result, these experiments are very valuable. Nevertheless, the experimental set-up can be considered to be small-scale and less severe than many accidents and real-life situations. Future large-scale data of this type can be valuable to confirm ability to predict real accident scenarios and further validation of risk assessment methods.

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