NUMERICAL SIMULATIONS OF A LARGE HYDROGEN RELEASE IN A PROCESS PLANT

Sommersel, O.K.[1,2] **and Bjerketvedt, D.**[1]
[1]**Department of Technology, Telemark University College, Kjølnes Ring 56, Porsgrunn, NO-3918, Norway**
[2]**Current address: StatoilHydro, Research Centre, NO-3908 Porsgrunn, Norway,**
olsom@statoilhydro.com

ABSTRACT

This paper describes a series of numerical simulations with release and ignition of hydrogen. The objective of this work was to re-investigate the accidental explosion in an ammonia plant which happened in Norway in 1985 with modern CFD tools. The severe hydrogen-air explosion led to two fatalities and complete destruction of the factory building where the explosion occurred. A case history of the accident was presented at the 1.st ICHS in Pisa, 2005.

The numerical simulations have been performed with FLACS, a commercial CFD simulation tool for gas dispersion and gas explosions. The code has in the recent years been validated in the area of hydrogen dispersion and explosions.

The factory building was 100 m long, 10 m wide and 7 m high. A blown-out gasket in a water pump led to release of hydrogen from a large reservoir storing gaseous hydrogen at 3.0 MPa. The accident report estimated a total mass of released hydrogen between 10 and 20 kg. The location of the faulty gasket is known but the direction of the accidental release is not well known and has been one of the topics of our investigations. Several simulations have been performed to investigate the mixing process of hydrogen-air clouds and the development of a flammable gas cloud inside the factory building, resulting in a simulation matrix with dispersions in all axis directions. Simulations of ignition of the different gas clouds were carried out and resulting pressure examined. These results have been compared with the damages observed during the accident investigation.

We have also performed FLACS simulations to study the effect of natural venting and level of congestion. The height of the longitudinal walls has been varied, leading to different vent openings at floor level, at the ceiling and a combination of the two. This was done to investigate the effects of congestion with regards to gas cloud formation.

The base case simulation appears to be in good accordance to the observed damages from the accident. The simulations also show that the build up of the gas cloud strongly depends on the direction of the jet and degree of ventilation. The CFD study has given new insights to the accident and the results are a clear reminder of the importance of natural venting in hydrogen safety.

INTRODUCTION

The use of hydrogen for industrial and commercial purposes is strongly linked to safety. Unintended leaks of hydrogen gas may cause fires and explosions, and research on safety is one of the key topics on the road to a hydrogen society. This includes both studies on dispersions and explosions. Amongst the present studies of the dispersion of hydrogen gas are the work by Swain and Swain [1] and Matsuura et.al [2]. Experiences from hydrogen related accidents are important contributions, such as Venetsanos et.al [3] and Bjerketvedt and Mjaavatten [4].

This paper describes a series of numerical simulations with release and ignition of hydrogen. The objective of this work was to re-investigate the accident in an ammonia plant (N1) which happened in Norway in 1985 with a modern CFD tool. The severe hydrogen-air explosion led to two fatalities and complete destruction of the factory building where the explosion occurred [5]. The accident report states that the event started when a gasket in a water pump was blown out. The pump was feeding water to a vessel containing hydrogen gas at a pressure of 3.0 MPa. The overpressure caused a back flow of water through the pump and out through the failed gasket. The hydrogen gas reached the leakage point after about 3 minutes. The gas discharge lasted between 20 and 30 seconds before the explosion occurred, with a total mass of hydrogen estimated at 10 to 20 kg. The main explosion was very violent, and it is likely that the gas cloud detonated. A complete case history of the accident was presented at the 1.st ICHS in Pisa, 2005 [4].

The numerical simulations have been performed with FLACS, a commercial CFD simulation tool for gas dispersion and gas explosions [6]. The code has in the recent years been validated in the area of hydrogen dispersion and explosions. FLACS has been used in several safety studies, among them work performed by Middha and Hansen [7, 8].

NUMERICAL SIMULATIONS SETUP

The numerical setup is based on the accidental report [5] and over 1000 pictures from the accident investigation team. The outlines of the geometry have been modelled as close to the real factory as possible. The findings from the investigation have been the basis of input to our simulations, for example the jet details and ignition source location. Each scenario was first simulated as a dispersion, and then ignited. Each case has therefore 2 coupled simulations.

We will present four scenarios in this paper. Case 1 is our base case, which gave results closest to the accident scenario. Case 2 represent a jet release directed horizontally towards one of the long sidewalls, and is used for comparison. Case 3 is simulations with vent openings in the longest side walls, with a 1 m opening in the longitudinal direction at the floor and ceiling. The last case is a simulation with no walls.

Geometry description

The inner dimensions of the factory building was 100 m long (x), 10 m wide (y) and 7 m high (z). The walls and roof were made of reinforced concrete elements. The roof was supported by several concrete support beams, placed at an interval of approximately 8 m throughout the length of the building. The support beams were 1 m wide. The main process equipment consisted of water pumps A and B, two motors, A and B and a row of turbines. The water entered the pumps through pipes from the long south wall. Other equipment was not modelled. A large garage door placed in the north wall, were open. A photo of the factory building after the accident is shown in Fig. 1.

Figure 1. Photo of the factory building after the accidental explosion, taken by the investigation team photographer [5]. The photo shows the northern wall

Our CFD geometry model is shown schematically in Fig. 2, exported from the FLACS pre-processor CASD, as a wire frame image. The ignition point was located at the base of pump A, at 1.0 m above the floor. The accident report concluded that the ignition most likely had happened due to a hot bearing in the driveshaft of this pump. The ignition point was positioned in the direction perpendicular to the jet, in order to get the simulated gas cloud ignited.

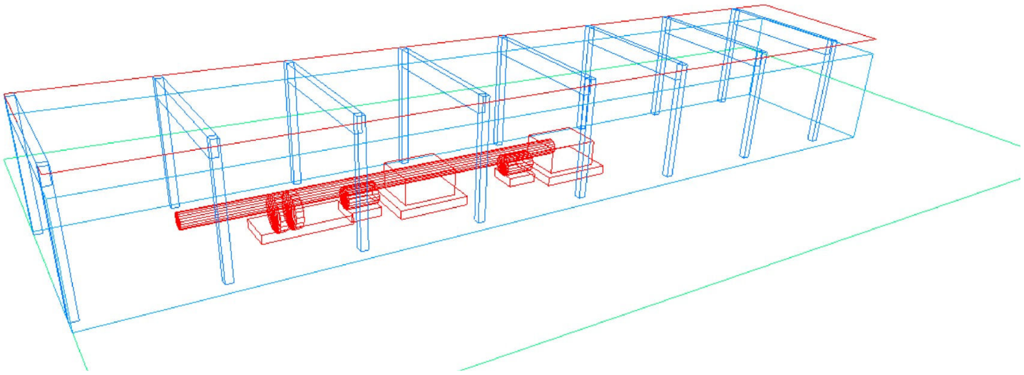


Figure 2. FLACS model of the N1 factory building

Simulation description

A series of FLACS simulations have been performed on the abovementioned geometry. The jet direction was varied, in an effort to find the most likely dispersion scenario that happened in the accident. We have also performed FLACS simulations to study the effect of natural venting and level of congestion. The height of the longitudinal walls has been varied, leading to different vent openings at floor level, at the ceiling and a combination of the two. This was done on the case with the results closest to the accident to investigate the effects of congestion with regards to gas cloud formation.

Table 1 show the simulation matrix. The initial fuel in the rightmost column describes the initial amount of fuel loaded from the corresponding dispersion simulation and into the ignition simulation. These values vary, because of the dilution of hydrogen in the surrounding air in the different scenarios. In case 4, the initial fuel is lower because the walls are removed so that the hydrogen gas exits the computational domain.

Table 1. FLACS simulation matrix

Case	Simulation details	Wall details	Initial fuel [kg]	p_{max} [kPa]
1	Release, +x	Solid walls		
	Ignition, +x	Solid walls	14.0	360
2	Release, -y direction	Solid walls		
	Ignition, -y direction	Solid walls	14.8	60
3	Release, +x direction	1.0 m opening, top and bottom		
	Ignition, +x direction	1.0 m opening, top and bottom	12.1	10
4	Release, +x direction	No walls		
	Ignition, +x direction	No walls	9.94	1

Jet details

The opening of the accidental release was 6 cm^2. The hole was a blown-out section of a gasket in a water pump, which led to a sector-shaped release. Parts of the jet hit a small steel pipe.

In our simulations, the jet inlet has been calculated in the corresponding jet utility program in the FLACS software package. Table 2 shows the input variables chosen for the calculations. Calculations from such an input-file provide a set of data, including Mach number calculations and effective nozzle diameter. The data is presented as a table, where effective nozzle area [m²], mass rate [kg/s], velocity [m/s] and temperature [K] among others, are listed for successive time-steps. The jet calculation output data set is loaded by the FLACS programme during the simulations to provide a time-dependant leak.

The reservoir volume was chosen to make sure that the reservoir pressure was treated as a constant, as the value of the reservoir volume was unknown. The accident report concluded that the pressure was 3.0 MPa prior to the accident.

The nozzle diameter was calculated from the assumption that the release opening area was 6 cm^2, and adjusted to represent a diameter in a spherical opening. The discharge coefficient was chosen to 0.63, based on the guidelines in the FLACS software manual. Based on the different simulation scenarios, the direction of the jet was changed accordingly. The relative turbulence intensity level was 0.2 in all the calculations. Heat transfer coefficients and wall temperature were 0.

Table 2. Jet calculation details.

Jet variables	Comments
10000	Reservoir volume (m^3)
3.0, 10	Reservoir pressure (MPa g) and temperature(°C)
0.1, 20	Atmospheric pressure (MPa a) and temperature (°C)
0.027639	Nozzle diameter (m)
0.63	Discharge coefficient (-)

Grid details

Cases 1 and 2 were run with a simulation volume of 0-50 m in x-direction, 0-10 m in y-direction and 0-7 m in z-direction. This corresponds to the walls of the geometry, and was chosen to minimize computational time. Cases 3 and 4 were run with a simulation volume of 0-55 m in x-direction, -5-15 m in y-direction and 0-10 m in z-direction. The Cartesian grid resolution was standardized to 0.2 m grid cells in all directions, and was stretched 5 % in the outer parts of the simulation volume. A grid sensitivity analysis has been carried out to verify the chosen grid size. Around the jet inlet, the grid were refined to 0.1 m, and smoothened to 0.2 m, 4 control volumes from the inlet. The grid was not refined in the direction of the jet.

NUMERICAL RESULTS

Our base case, Case 1, gave reasonable dispersion results compared to the accident. The jet hit the casing of pump A in less than 0.1 seconds, and the gas was diverted in a spherical manner. Some of the gas was directed outwards, hitting the side walls and creating a horizontal circulation zone. Most of the gas was then forced upwards, caused by the concrete foundation of the pump acting as a diversion. As the gas reached the ceiling, it was directed outwards in all directions. Because of the concrete support beams located under the ceiling, the gas was forced downwards along the side walls of the beams, in addition to the longitudinal walls. This created a large recirculation zone, both in the x- and y-directions. The recirculation zone was fed even more by the powerful jet in a forced feedback loop. After approximately 6.8 seconds, the flammable hydrogen gas reached the top level of engine A, and after 20 seconds the volume between the ceiling and the floor mounted equipment was above 15 percent. The concentration level at the drive shaft connecting engine A with pump A (1 m above floor) reached 12-15 percent after 20 seconds. The accident report concluded that a red hot bearing in the drive shaft of this pump was likely the ignition source. Fig. 3 shows the concentration contours in a cut plane in the centre (longitudinal) of the building after a 20 s release. Our dispersion results in this

FLACS simulation may confirm this, both the location and the time of ignition after the release started seems reasonable.

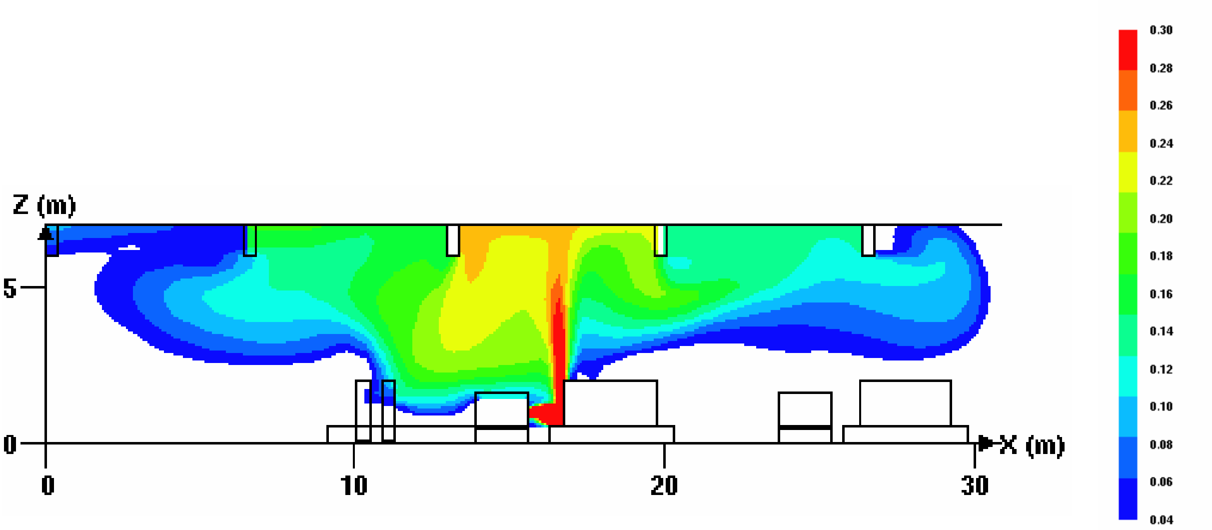


Figure 3. The figure shows concentration contours in a cut plane in the centre (longitudinal) of the factory building after a 20 s release. The jet hits a motor casing, forcing the gas upwards. Support beams under the ceiling create a recirculation zone. Colours indicate a range of concentrations from 0.04 (dark blue / > LFL) to 0.3 (red / > stoich.). White regions indicate a concentration of less than 0.04 (not flammable / < LFL).

The ignition of the gas cloud in Case 1 gave high explosion overpressures. The monitor located directly above the jet (M7) recorded a maximum explosion pressure of 210 kPa. One monitor located close to the lower southeast corner of the building gave a maximum of 360 kPa (M1) and recorded the highest maximum overpressure in this simulation. The pressure records of the monitors M1 and M7 in Case 1 are shown in Fig 4.

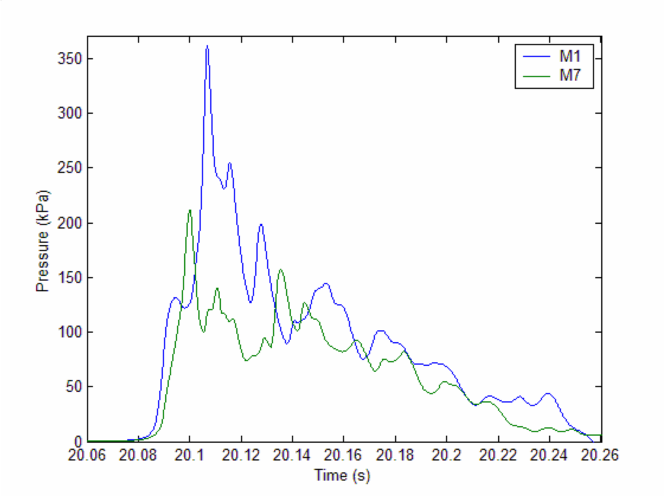
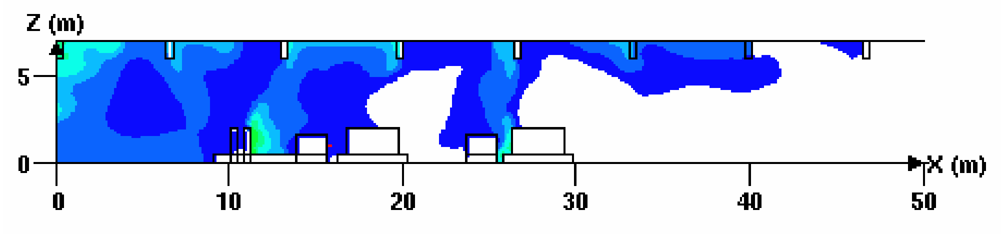


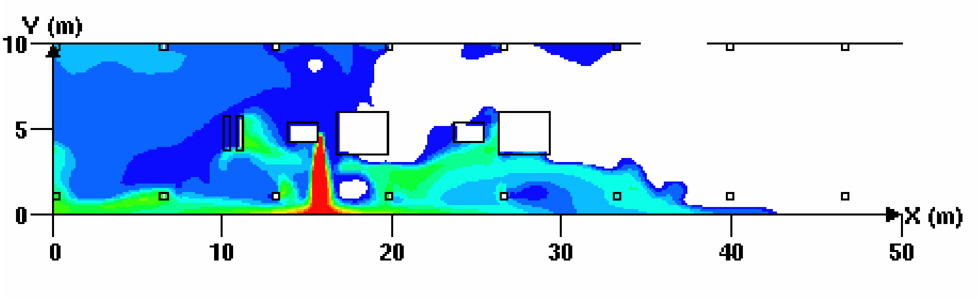
Figure 4. Case 1 pressure records from monitors M1 and M7

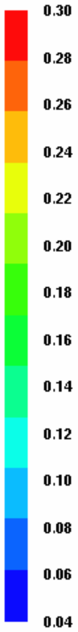
Simulations with the jet release directed vertically upwards (+z) gave results similar with Case 1, but with even stronger recirculation zones. The explosion overpressures in this simulation were also comparable.

Case 2, which had the release directed towards one of the long sidewalls, gave a significantly different result than Case 1. The hydrogen gas hit the wall, and was directed to the sides and upwards. The length of the gas cloud was longer than in Case 1, and the development of the cloud was not as controlled by large recirculation zones. The hydrogen concentration in the mixture was lower than in Case 1. Fig 5a shows the concentration contours from simulations on Case 2 in a side view cut plane in the centre (longitudinal) of the building after a 20 s release. Fig 5b shows the concentration contours from top view, in the height of the release (1 m). Pressure records from the explosion simulation show a maximum over-pressure of about 50 kPa. Monitors M1 and M7 are shown in Fig 7, where M1 recorded the highest maximum overpressure in this case.



a) Side view





b) Top view

Figure 5. Case 2. The figure shows concentration contours in cut planes along the x-axis after a 20 s release. a) side view cut plane in the centre (longitudinal) of the factory building, b) top view cut plane at the height of the release (1.0 m) Colours indicate a range of concentrations from 0.04 (dark blue / > LFL) to 0.3 (red / > stoich.). White regions indicate a concentration of less than 0.04 (not flammable / < LFL)

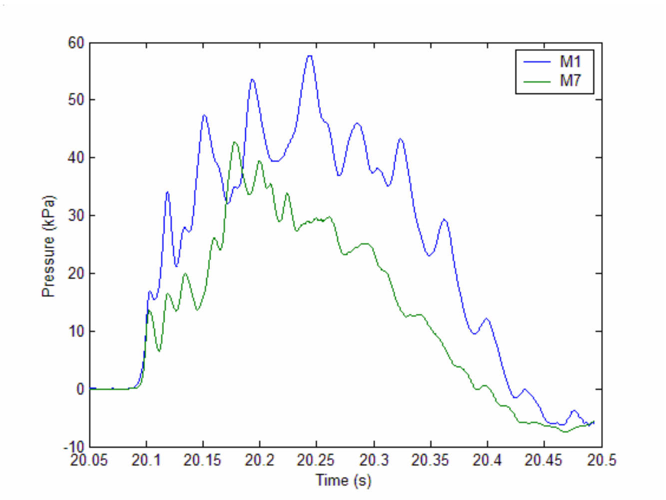


Figure 6. Case 2 pressure records from monitors M1 and M7

Case 3 was performed to investigate how passive ventilation would work in this geometry. The length-wise openings along the floor and ceiling vented some of the gas out of the building. One of the main advantages with this geometry was that the mean hydrogen concentration was lowered from about 20 % in the comparable Case 1 to about 15 % in Case 3. Figures 7 and 8 show the concentration contours in cut planes located 0.5 m from the jet nozzle, i.e. between the nozzle and pump A.

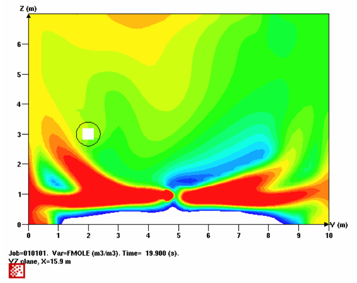


Figure 7. Case 1 concentration contours in a cut-plane 0.5 m from the jet (x-direction)

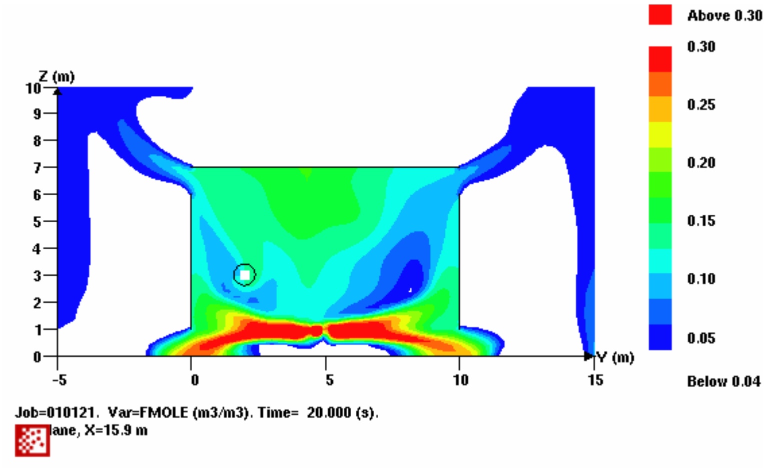


Figure 8. Case 3 concentration contours in a cut-plane 0.5 m from the jet (x-direction)

Case 3 yielded a relatively small gas cloud located under the factory ceiling. The behaviour of such releases has been reported in Hansen and Middha [8] and in Sommersel et.al [9]. The explosion simulation of Case 3 gave relatively low explosion overpressures, compared to our base case. The highest maximum was 10 kPa, recorded in M2 located close to the northern side wall at level with the jet location.

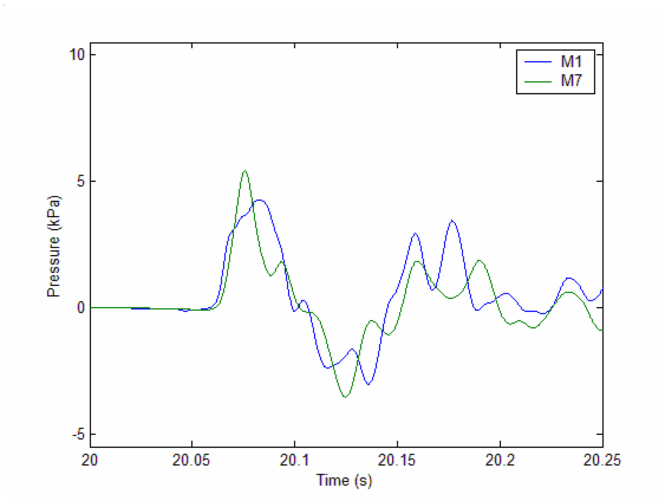


Figure 9. Case 3 pressure records from monitors M1 and M7

FLACS simulations on the factory building without walls were performed to study the development of a hydrogen-air mixture in a more open environment. Originally, the factory was designed without walls as a safety precaution. Due to the cold Norwegian winter climate, the walls were added at a later stage to prevent the water inside the building to freeze. The results from simulations on Case 4 show that the hydrogen is effectively vented out of the building, and the potential for an explosion have been dramatically reduced. Fig. 10 shows the concentration contours in the centre of the building.

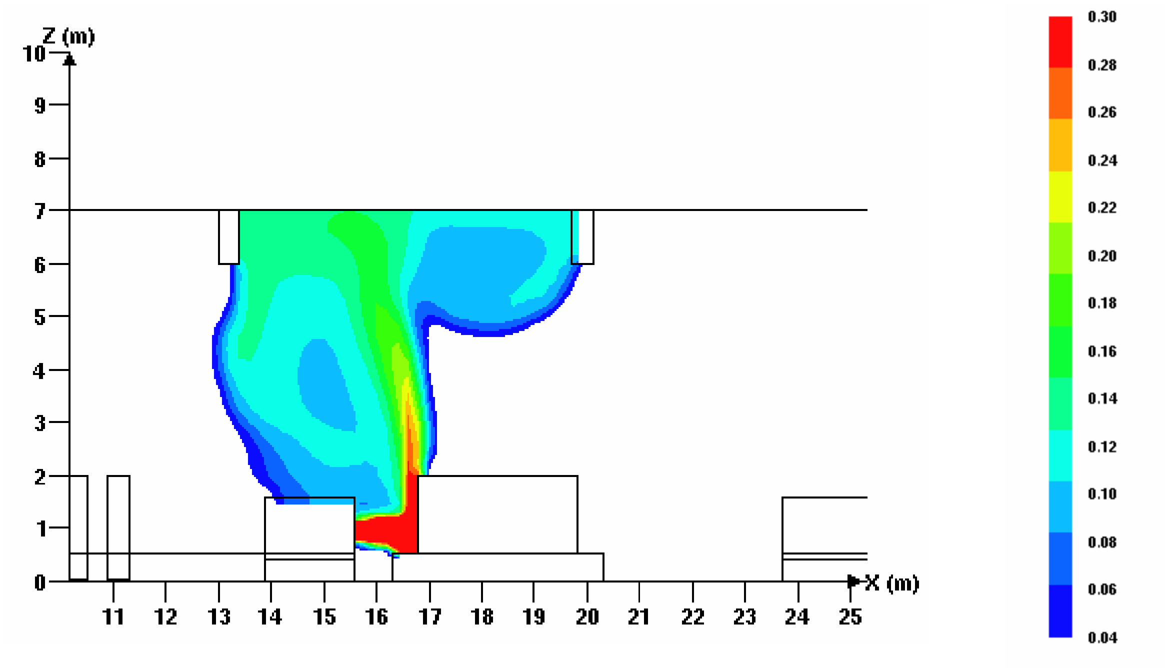


Figure 10. Concentration contours in a cut plane in the centre (longitudinal) of the factory building after a 20 s release. The jet hits a motor casing, forcing the gas upwards. The gas then gets forced to the sides and out of the building. Colours indicate a range of concentrations from 0.04 (dark blue / > LFL) to 0.3 (red / > stoich.). White regions indicate a concentration of less than 0.04 (not flammable / < LFL).

The consequence of removing the walls is shown in Fig 11, where concentration contours in a volume plot shows the effective venting of the hydrogen-air mixture in the factory building without walls. This case was impossible to ignite at the same location as the other three cases reported here, indicating that the explosion would probably not occur in this geometry layout. This case was ignited with the ignition located above the release close to the ceiling, in the centre of the factory. The maximum overpressures were in the order of 1 kPa.

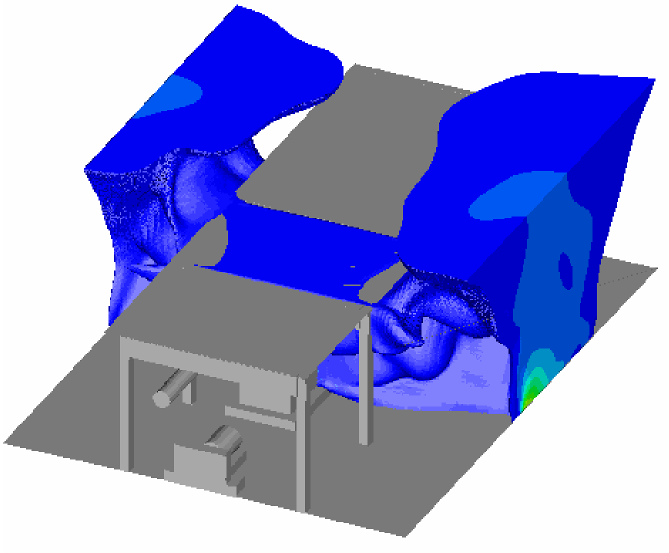


Figure 11. Concentration contours in a volume plot shows the effective venting of the hydrogen-air mixture in the factory building without walls (Case 4). Colours indicate a range of concentrations from 0.04 (dark blue / > LFL) to 0.3 (red / > stoich.). White regions indicate a concentration of less than 0.04 (not flammable / < LFL).

DISCUSSION

The simulations show that the dispersion is very sensitive regarding the changes in the jet direction. Obstructions in the jet changes the gas cloud formation dramatically, compared to a free jet. This corresponds well with our results from experimental tests performed in 2005 [10], where one of the tests was carried out with a hydrogen jet hitting an obstacle located only 0.2 m from the nozzle.

The ignition source was reported to be a red hot bearing, which we consider to be a weak ignition source. Would a hot plate like this be sufficient to ignite a hydrogen-air mixture containing 12-15 % hydrogen? The time of ignition is surely a topic for discussion, given that the report assumes the time of ignition to be an interval between 20 and 30 seconds. We have only reported simulation cases with 20 s release in this paper, but a comparison of results from both 20 and 30 s releases would be rewarding as a part of further work on this topic.

The accidental report does not contain a clear direction of the release, and to our understanding the release have had to be some kind of sector-shaped release. In our FLACS simulations we have assumed that the jet release was directed along one of the axes only, which perhaps is too conservative.

Simulations on the factory building without walls show that 'the best building has no walls', as stated by Trevor Kletz [11]. The hydrogen-air mixture was effectively vented to the outside of the building, reducing the probability for accidents by a large degree. Also in this case, the explosion overpressures were small.

It has to be taken into account that the FLACS code calculates deflagrations only. Results from our explosion simulations will therefore have a degree of uncertainty, when compared with the N1 accident. It is likely that the gas cloud detonated, as stated in the accident report. However, the use of the FLACS CFD tool have shed some light on how the accident may have happened, and have certainly given new insights in understanding the gas cloud formation that occurred in the accident.

CONCLUSIONS

The simulations show that the dispersion is very sensitive regarding the changes in the jet direction.

The results from the simulations with solid walls are in good accordance to the observed damages from the N1 accident.

The FLACS code calculates deflagrations only, so our results from the explosion simulations will therefore have a degree of uncertainty, when compared with the accident. The use of the FLACS CFD tool have shed some light on how the accident may have happened, and have given new insights in understanding the gas cloud formation that occurred in the accident.

ACKNOWLEDGMENTS

Financial support from the Norwegian Research Council Programs, Strategiske høgskoleprogram and RENERGI, is gratefully acknowledged.

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