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CFD-modelling of Large-scale LH2 Release Experiments

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As a part of zero emission ambitions within the maritime, and possibly within aviation, liquid hydrogen (LH2) will increasingly be used as fuel in the coming years. In that respect it is important to understand safety aspects of LH2, including gas dispersion and explosion properties. The Norwegian Public Roads Administration commissioned large-scale LH2 dispersion and explosion experiments both indoor and outdoor when developing their first LH2-fuelled ferry. In this article these experiments are simulated using a CFD-model with the aim to validate a modelling approach for gas dispersion from LH2-releases.

1. Introduction

The Norwegian Public Roads Administration have ambitions to decarbonise all their 126 ferry connections with more than 200 ferries in the coming years. Around 55 of these are electrified at end of 2021, and an estimated 70 electric ferries are expected in operation by the end of 2022. Realising that some ferry connections are challenging to electrify, NPRA held a tender in 2018 to build and operate a hydrogen ferry using LH2 as a fuel. Ferry company Norled won the tender, and the ferry MF Hydra has been built and has entered operation this year, so far only as a battery electric ferry. The hydrogen operation is expected to start Q1 2022 once the permitting process is completed.

The use of LH2 in Europe is limited and there is currently no LH2 production north of Germany. As there is no experience handling LH2 at industrial scale in Norway, and quite limited experience elsewhere, NPRA decided there was a need to perform large-scale experiments to build knowledge. Two test series were performed and completed early 2020 at the DNV Spadeadam test site, studying both large indoor and outdoor releases. NPRA made the test report from DNV publicly available, see Medina and Allason (2020) and Medina et al. (2020), and the Norwegian Defence Research Establishment (FFI) who coordinated the test activity on behalf of NPRA also published a report (Aaneby et al., 2021).

The outdoor release experiments were significantly better instrumented than the previous important largescale tests by AD Little (1960) and NASA (Witcofski and Chirivella, 1984) with field gas detection 30 m, 50 m and 100 m away. The tests are also considered more realistic for the understanding of incidents related to a vessel bunkering situation as directed releases downwards and horizontally from a bunkering line at overpressure were studied. While extensive data sets exist for validation of LNG-dispersion models, see (Hansen et al., 2010), less relevant data exist for LH2. The NPRA data thus represents very valuable validation data for CFD-modelling approaches of vapour dispersion from LH2-spills and is used to validate the LH2-vapour modelling approach described by Hansen (2020). In previous experiments by NASA and BAM, see (Statharas et al., 2000), special nozzle release arrangements were constructed to obtain and study LH2pool spread not considered so relevant for the typical vessel bunkering situations. In the NPRA tests flammable LH2-vapour plumes were also ignited to study flame acceleration and explosion pressures.

The indoor experiments assessing large LH2 releases inside a container were meant to simulate a vessel tank connection space. While the large release rates studied should in our opinion by design never be allowed to happen, the tests gave several interesting results related to LH2 spills, gas dispersion, air entrainment and explosions in cold LH2-vapour and air. As described by Hansen (2020) only very small LH2 releases which can be managed safely by ventilation should be possible inside the TCS, all larger leaks must be contained safely in double piping and led to gas mast. Due to the very high reactivity of LH2-vapour, indoor leaks that can give explosive concentrations must be prevented, alternatively an uncontrolled situation with LH2-vapour detonation potentially damaging the LH2 storage tank or connections could be feared.

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2. Simulation of outdoor LH2 release experiments

Seven different experiments were performed as part of the outdoor LH2 release experiments, three of the tests had a character of preparatory tests or final test with the aim to empty tanks, while tests 3 to 6 were near identical repeats of two different scenarios. These are described below.

2.1 Overview of outdoor LH2 release experiments

Test 5 was a release from 1" (25 mm) orifice from 2" (50 mm) tanker pipe downwards 0.32 m above the concrete ground with leak rate 0.74 kg/s and wind speed around 4 m/s, while test 3 was a similar release test with slightly higher wind speed and lower release rate. Test 6 was a horizontal release along the wind 0.50 m above ground with leak rate around 0.83 kg/s, with wind speed around 2.5 m/s. Test 4 was similar to test 6 but with somewhat stronger winds. The duration of the different tests were 3 to 15 min and tests 5 and 6 were ignited once a steady LH2-vapour plume had developed. As is often the case for outdoor experiments there is a significant variation in wind speed and direction with time. In the test setup there were gas detectors at 5 locations in the 30 m arc, 3 locations in the 50 m arc and only 2 locations at 100 m distance. When comparing CFD-simulations to experiments, the maximum concentrations (minimum temperatures) predicted at a given distance should be compared to the short-term maximum concentration observed in the experiment. In some cases, the plume in the experiment may fail to properly expose a detector array and reported plume concentrations may be too low. In addition to gas/temperature detectors there were 5 detectors to report pressure waves from the ignited plumes, thermal detectors to report low temperatures in the concrete below the release, and radiation sensors for fire after ignition. In Figure 1 the plume of fog (condensed air humidity) from the experiment is visually compared to the predicted hydrogen contour around 50% LFL for the 0.74 kg/s downwards release, for both cases a clear bifurcation of plume can be seen (two ridges). Some details of the different experiments are shown in Table 1.



Test	Leak	Leak rate	Wind Average	Range	Direction	Reported temperature	Assumed humidity
3	0.32 m down	630 g/s	5.1 m/s	-0.2-13.4 m/s	101-317 deg	3.0 °C	
4	0.50 m along wind	828 g/s	5.8 m/s	1.3-12.1 m/s	223-331 deg	4.0 °C	
5	0.32 m down	739 g/s	4.3 m/s	-0.6-9.1 m/s	231-306 deg	4.0 °C	90%
6	0.50 m along wind	833 g/s	2.5 m/s	0.5-5.8 m/s	191-317 deg	4.0 °C	90%

2.2 Simulations and comparison with experiments

LH₂ releases were simulated with the FLACS CFD-model following the modelling approach described by Hansen (2020). The LH2 outflow velocity was estimated using Bernoulli equation and pressure reported near the outflow location (P4 – typical pressure level of 230-250 kPag). In the pseudo-source modelling with some limited air entrainment an initial flow velocity around 70 m/s was assumed. In Table 2 predicted gas concentrations and temperatures from the simulations at distances 30 m, 50 m and 100 m were compared those reported from the experiments. In Figure 2 concentrations and temperatures predicted at ground level are shown for both tests. For the 739 g/s downwards release the plume spreads well laterally and exposes gas detectors at all measurement arcs in the experiment. The predicted concentrations corresponded quite well with the experiments with near 8% concentration at 30 m distance and almost 4% at 50 m. Due to the significant average wind speed around 4.3 m/s, hydrogen concentrations are reported near the ground in the 100 m arc. For the 833 g/s horizontal release along the wind direction a much narrower plume with higher concentrations are around 8% while the reported concentrations are much lower, around 2%.

The reason for this deviation is likely that the narrow plume in the experiments mostly missed the three detectors of the 50 m arc. In the 100 m arc neither the simulation nor the experiment reported any hydrogen concentrations. For the simulation this was caused by a plume lift-off around 70-80 m from the release, due to reduced concentrations and low wind speeds. Such lift-off is expected for LH2-vapour dispersion at lean concentrations in low wind due to air humidity, see (Hansen, 2020) and (Giannissi and Venetsanos, 2018), and this effect is clearly seen in the NASA-tests. Plume temperatures tend to correlate well with hydrogen concentrations. For the high wind scenario, the predictions corresponded well with test reports, while for the scenario with less wind the predicted plume was slightly colder than the reported plume, this could be due to heat transfer from the ground to the plume. Benchmarking against atmospheric releases is often very challenging due to wind variations and quality of data, see e.g. (Hanna et al., 2004). With this in mind the correlation between experiments and simulations obtained above must be considered very good.

Previous LH2 spill experiments have focused on understanding pool spread. In the modelling approach it has been assumed that the released LH2 would immediately vaporize in contact with air, and that possible deposits, if any, would be frozen or condensed air. This assumption seems to have been confirmed by the experiments. For the downwards release of 739 g/s from 0.32 m elevation, temperatures below -200 °C in the concrete were only reported for detectors up to 0.5 m from the impinged release, and near -200 °C was only seen at a couple of detectors at 1 m distance, likely due to the downwind plume. The videos also gave no indication of any pool formation. For the horizontal release 0.5 m above ground the lowest temperature reported in the concrete was around -20 °C.

Test Leak direction		Wind	Distance	Concentration		Temperature	
				Experiment	Simulation	Experiment	Simulation
5	739 g/s down	4 m/s	30 m	7.6%	~7%	-8.5°C	-9°C
			50 m	2% (T3: 3.5%)	3.5%	-2°C	-3°C
			100 m	1.5%	2.0%	Not readable	0°C
6	833 g/s along wind	2.5 m/s	30 m	21%	22-23%	-35°C	-50 °C
			50 m	2% (missed arc)	8%	-2°C (T4: -13°C)	-20 °C
			100 m	No recordings	Plume lift-off	No recordings	Plume lift-off

Table 2	: Experiments	and simu	lations c	ompared.
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Figure 2: Ground level predicted hydrogen volume fraction (left) and temperature (right) for test 6 with horizontal release in 2.5 m/s wind (upper) and test 5 with downwards release in 4 m/s wind (lower).

In the downwards release experiment test 5 there was an attempt to ignite the plume at 24 m distance by sprays of sparks but with no success. A second attempt to ignite at 18 m distance was successful with flame burning back to release and into the other half of the bifurcated plume. The simulated plume was also ignited, with ignition at 18 m the plume ignited but was unable to burn back to source due to the low concentrations and significant wind. By moving ignition to 15 m from the release the flame accelerated back to the source. For 5 out of 6 pressure sensors the predicted maximum pressures in the simulation corresponded well with the pressure level from the experiments (1.5 kPa) except for one pressure sensor in the simulation reporting 4

kPa. The horizontal release was ignited at 30 m distance and gave a strong flame acceleration back to source, see simulated explosion in Figure 3. Explosion pressure in the experiment and the simulation were consistent ranging from 2-3 kPa for the one sensor reporting the highest pressure to 1.2 kPa and below for the other 5 pressure sensors. While these pressure levels would not be of particular concern for a bunkering situation the flame speeds were high and there could be situations with gas trapped in more confined areas which could give strong explosion pressures in a practical situation, e.g. if cold LH2-vapour gets trapped between the ship and the quay. This can be assessed with CFD-calculations.



Figure 3: Test 6 was ignited at 30 m distance which led to a strong flashfire back to release.

Another interesting observation from the videos is that the flame of test 5 stopped propagating outwards well before the 30 m arc. This was expected as only upwards propagation should be seen for concentrations below 8%. This aspect is important to consider for LH2 bunkering assessments.

3. Simulation of indoor LH2 releases

A test campaign with large LH2 releases inside a ventilated container with a vent stack was also performed. This setup was defined to simulate releases in a vessel tank connection space (TCS) which is a room directly connected to the LH2 fuel tank where LH2 is vaporized and heated to ambient temperature before being sent to the fuel cells or combustion engines at an overpressure around 500 kPa. For LNG, TCS piping may be single, and leaks may flow directly into the TCS which is meant to be a well-ventilated secondary barrier. If so, an explosion could happen but due to the low reactivity of cold LNG-vapour and stratification effects, no severe explosion would be expected. For LH2, main piping would need vacuum (or helium) insulated double piping to prevent air condensation outside piping. Large releases would further not be tolerable due to the high reactivity of LH2-vapour mixed with air as an explosion could well undergo DDT and detonate with potentially severe consequences to the tank and connecting piping. As suggested by Hansen (2020), LH2 leaks into the TCS should be limited to 1-3 g/s, and all larger leaks must be collected by double piping and led safely to vent mast. Thus, the leak scenarios investigated as part of the indoor LH2 release campaign would be in conflict with such a safety strategy and should not be allowed. Still, there were some interesting findings from the experiments which will be discussed in the following.

3.1 Overview of experiments

The indoor LH2-release experiments included 8 different experiments. The first 5 experiments were dispersion only, with LH2 spills up to around 500 g/s downwards centrally onto the floor of a $3.0 \times 3.0 \times 2.3 \text{ m}$ (~20 m³) container with no or limited ventilation. The room had a $0.49 \times 0.50 \text{ m}$ ventilation opening near the floor on one side, a $2.3 \times 1.6 \text{ m}$ large explosion vent opening (55% by area) on the front wall, and a 3 m horizontal and 10 m vertical 450 mm diameter vent stack from the upper part of the wall opposite the ventilation inlet.

In these tests the temperature quickly fell below -200 °C inside the entire room and stack, and hydrogen concentration approached 100%. A pool of LH2 spread centrally on the floor 0.5-1.0 m from the release and there were also significant deposits of frozen air on the floor, in this area temperatures of -240 °C were reported, likely indicating presence of a pool. Within 30-40 s from the releases were stopped all the LH2 would have evaporated from the pool while it took a long time before the frozen air deposits would melt and evaporate. The last three experiments were particularly interesting as the cold hydrogen exiting on the top of the stack was ignited after a steady-state situation had developed. In test 13 the lower air vent opening was closed, and after the vent flow was ignited it took around 30 minutes before the flame managed to burn down into the stack to give a low severity explosion inside the container. This test is considered interesting related to hazards of hydrogen venting to vent masts if there is no inerting of the vent masts. Air will gradually entrain the vent mast, and after 30 min to a few hours there could be a strong explosion inside the vent mast. To prevent

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this inerting will be require either permanently or after a release to mast. In test 14 this setup was repeated except that the small ventilation opening near the floor of the container was kept open so that air would enter while the hydrogen flare burned at the top of the mast. The test report stated that it took only 10-15 s from ignition until a strong explosion with pressures around 200 kPa at monitor point inside the container, even if there was a very large vent panel in the front of the container. Test 14 is simulated and presented in the next section. Test 15 was also ignited but less interesting as ignition was performed at very fuel rich concentration.

3.2 Simulations and comparison with experiments

A FLACS CFD simulation studying the explosion of test 14 was performed. This is a very challenging test setup in which a very cold hydrogen gas cloud around -200 °C is ignited at the outlet of the stack with a flame burning at the top of the stack while air is pulled into the container through the passive vent opening. In Figure 4 simulation plots presenting hydrogen volume fraction (FMOLE) and temperatures 15 s, after ignition when flame starts to enter gas mast in simulation, and after 27 s, just before the flame reaches the 90 degrees bend of the stack and explodes into the container. At that time the hydrogen concentration inside the stack is between 60-70% while the lower half of the container is at highly reactive concentrations between 30-50% hydrogen and temperature -30 to -50 °C. Explosion overpressures at the monitor locations inside the container were predicted from 150 to 180 kPa in the simulation and 130 to 230 kPa in the experiment with duration 20-30 ms in both cases, see Figure 5. Observed and predicted flames are also shown.



Figure 4: Hydrogen mole fraction (FMOLE) and temperature 15 s after ignition on top of the vent stack (left) and 27 s after ignition just before flame shoots into the container and explodes (right).



Figure 5: Explosion pressures inside container reported from experiment 14 (left) and predicted in simulation (right), lower plots show external flame from test and simulation.

The high overpressures above 200 kPa resulted despite a non-optimal gas concentration and the light pressure relief panel covering 55% of the front area of the container. With a lower leak rate of the order 30-50 g/s rather than 500 g/s, a much more homogeneous gas concentration resulting in significantly higher overpressures should be feared if ignited. As most TCSs will be more confined such scenarios would lead to severe destruction of the TCS, which is one reason for the recommendation not to tolerate significant leaks of LH2 into the TCS.

4. Conclusions

NPRA performed interesting large-scale LH2 release tests at DNV test site Spadeadam to build confidence and understanding related to handling of LH2 as fuel on ships. One test series with outdoor releases of 700-800 g/s relevant for LH2 bunkering incidents is considered particularly valuable for validation of LH2-vapour dispersion, with gas concentration and temperature measurements reported at distances 30 m, 50 m and 100 m from the releases. Predictions from FLACS CFD simulations of these experiments, using a pseudo-source approach for the near field correlated very well with the experimental results, and substantiates that LH2release dispersion can be predicted with reasonable confidence. Explosion simulations in the dispersed vapour clouds also gave very similar predicted overpressures to those observed in the experiment. Other important and interesting observations from these experiments include the observation that no LH2 pool formation was observed despite release of 740 g/s directed downwards onto the ground from 0.32 m elevation and that plumes were denser than ambient air at reactive concentrations. High flame speeds were also seen at reactive concentrations in unconfined vapour clouds, and as expected the reactivity was very low for plumes below 8-10% concentration. For one of the simulations with limited wind (2.5 m/s) the predicted plume seems to have lifted off the ground after 70-80 m, the fact that no gas was reported in the 100 m arc in the experiment may be a result of a lift-off also of the plume in the experiment. Experiments were also performed with large releases (~500 g/s) inside a container representing a vessel tank connection space (TCS). Such a release into air would be considered to lead to an unsafe situation with potential for DDT and detonation in the vicinity of the LH2 tank and should not be considered acceptable. Still, there were interesting findings from the experiments, both related to the ability of a flame gradually to burn back into a vent mast filled with cold hydrogen, and not least the high explosion pressures seen inside the TCS.

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