HyApproval

WP4 - Safety

Preparation of simulation for selected accident scenarios
Agreement on prerequisites for numerical safety analysis

Deliverable 4.6

- PUBLIC -

Agreement on required modelling tools & techniques for risk assessments and simulations, accident scenarios, credible leak rates

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1 Introduction

Deliverable D4.6 is intended to summarize the agreement between partners participating in WP 4 – Safety on numerical tools, techniques and the data necessary to perform safety analysis of relevant accident scenarios. The codes and techniques can include both multi-dimensional CFD programs and simplified tools for integral evaluation of possible consequences and damages. The data necessary for safety analysis consists of set of credible scenarios, which has to be analysed, complemented by corresponding initial and boundary conditions.

2 Accident scenario selection for modelling

After intensive discussions within WP 4 (including two workshops dedicated to the development of scenarios selection methodology), the set of possible scenarios was formulated (see deliverable D 4.3). All these scenarios are listed in Table 2. Selected scenarios are separated into three groups depending on their possible hazard direction:

- external safety;
- customer safety;
- others (here were grouped the scenarios having potential for violation of both external and internal safety).

2.1 General approach to scenario selection

Preliminary analysis demonstrated that not all the scenarios require CFD modelling. Some of the scenarios can be analysed using simplified (integral) tools; some can be simply excluded from the list.

Consideration of the scenarios being the members of the group ‘customer safety’ permits to omit the group from candidates for numerical analysis. All these scenarios, excluding DL1, belong to the ones of minor hazard potential. The maximum release rates for hydrogen leaks for scenarios D6, D5, DL10 does not exceed 1 g/s (see Table 1).

Table 1 Data on mass flow rates for scenarios of ‘customer safety’ group

Scenario	Pressure	Leak size	Leak rate (g/s)	Leak rate (nm/s)
D5 minor leak	350 bar	0.1 mm	0.10 g/s	1.2 nm/s
D5 major leak	350 bar	0.2 mm	0.41 g/s	5.0 nm/s
D6 minor leak	700 bar	0.1 mm	0.17 g/s	2.1 nm/s
D6 major leak	700 bar	0.2 mm	0.70 g/s	8.3 nm/s
DL10 minor leak	8 bar	0.1 mm	0.003 g/s	0.04 nm/s
DL10 major leak	8 bar	0.2 mm	0.013 g/s	0.15 nm/s

It was shown earlier that in case of small leakages (e.g., Breitung *et al.*[1] simulation for private garage with leak equal to 0.34 g/s) the concentration of hydrogen does not

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[1] W. Breitung, G. Necker, B. Kaup, V. Veser. Numerical Simulation of Hydrogen Release in a Private Garage, The 4th Int. Symp. On Hydrogen Power – Theoretical and Engineering Solutions, Proceedings v. 2, 9 – 14 Sept. 2001, Stralsund, Germany, pp. 368 – 377.

reach high enough values, at which an onset of detonation is possible. Therefore, the mentioned above scenarios can be excluded from those requiring detailed consideration.

Note, that despite relative minor hazard potential of such accidents, the partners of HyApproval project can recommend to perform systematic analysis of small leaks with possible quantification of higher acceptable limits for mass flow rates and/or hydrogen inventories.

In case D3 ‘Leakage inside dispenser enclosure’, it is assumed that there is no accumulation of hydrogen since its interior is naturally ventilated.

All other scenarios require more detailed consideration since none of them could be excluded *a priori* as in case of small amounts and/or small releases. Note, that each of the remaining 10 scenarios includes several variants, such as: mitigated / non-mitigated scenario development, wind / no wind, storage pressure 35 / 70 MPa for compressed hydrogen, etc. The total number of cases can exceed 50 and cannot be analysed in their completeness in the frames of the current project.

Since the project DoW foresees calculations of about 15 cases only, the partners decided to share their work in accordance with their numerical capabilities, experience and relevant importance of selected for simulation scenarios.

Table 2 List of possible scenarios

Ref	**Description**	**External safety**	**Customer safety**	**Other**	**Phenomena**	**Non mitigated**	**Mitigated**	**Refuelling station class**	**Remarks**
D4	Rupture of dispensing line (flexible hose),	▨			Jet fire & explosion	YES	YES	Compressed 350 and 700 bar	Mitigation shall reduce release duration and quantity
S1	Rupture of H2 buffer storage output line,	▨			Jet fire & explosion	YES	YES	Compressed 350 and 700 bar	Mitigation shall reduce release duration and quantity
S8	Burst of hydrogen storage tank,	▨			Burst (overpressure) & missiles	Not applicable	Not applicable	Compressed 700 bar	Burst of one tank. Effect of protection wall to be considered.
PR1	Rupture of NG feed line inside production container,	▨			Explosion	Not applicable	Not applicable	Compressed	Explosive atmosphere inside container.
T1	Trailer hose disconnection during refilling	▨			Jet fire & explosion	YES	YES	Compressed 250 bar	Is likely to be more severe than D4. Mitigation shall reduce release duration and quantity
DL8	Shear of the hose line,	▨			Fire & explosion	YES	YES	Liquid 8 bar	Mitigation shall reduce release duration and quantity
TL1	Leakage after discharge when decoupling (hydrogen source not isolated),	▨			Fire & explosion	YES	YES	Liquid 11 bar	Is likely to be more severe than DL8. Mitigation shall reduce release duration and quantity
SL3	Below ground storage failure (with vault),	▨			Fire & explosion	YES	YES	Liquid 8 bar	Mitigation shall reduce release duration and quantity
D6	Leakage at nozzle during		▨		Explosion &	NO	YES	Compressed	

Ref	Description	External safety	Customer safety	Other	Phenomena	Non mitigated	Mitigated	Refuelling station class	Remarks
	refuelling,		▨		standing flame			350 and 700 bar	
D5	Hole in dispensing line		▨		Explosion & standing flame	NO	YES	Compressed 350 and 700 bar	
D3	Leakage inside dispenser enclosure		▨		Explosion	Not relevant	Not relevant	Compressed	
DL1	Leakage at nozzle during refuelling		▨		Explosion	NO	YES	Liquid 8 bar	
DL10	Hole in dispensing line		▨		Explosion	NO	YES	Liquid 8 bar	
S7	Release of hydrogen through vent line			▨	Explosion & jet fire	Not relevant	Not relevant	Compressed 350 and 700 bar	
SL1	Release of hydrogen through vent line (loss of vacuum)			▨	Explosion & jet fire	Not relevant	Not relevant	Liquid 8 bar	

2.2 Leak rates and hydrogen inventory in accident conditions

Since the hazard potential of the accident scenario is strongly dependent on leakage release and resulting total inventory of hydrogen, which can be involved into combustion and explosion process, these data are extremely important for the accident scenario evaluation and ranking.

Based on long-term experience of industrial partners involved in the HyApproval project, the knowledge of possible leaks, details of mitigation measures and expertise in refuelling technique and equipment permitted to define credible required initial and boundary conditions for the selected scenarios. Typical data which are necessary for calculations (excluding geometrical layout configurations) are the following:

- mass flow rate of the leak;
- size (diameter for pipe ruptures) of the leak;
- internal pressure of the leaking vessel or mass velocity at the opening;
- time of isolation for mitigated scenarios;
- data or indications on hydrogen inventory;
- peculiarities of leak, e.g., flow obstructions, flow direction, active or passive ventilation, etc.
- ambient conditions, i.e. wind speed and wind direction

Results of leak details for the selected scenarios are summarized in Table 3.

Table 3 List of accident scenarios, data required for simulations and leakage data

Ref	Description	Phenomena	Non mitigated	Mitigated	Necessary data	Input from Industry
D4	CGH2 dispenser: Rupture of dispensing line (flexible hose),	Jet fire & explosion	YES	YES	▪ Hose internal diameter ▪ Time for isolation (mitigated scenario) ▪ Inventory to be released	35 MPa ▪ 6 mm ID for cars; 11 mm ID for buses ▪ Isolation within 2 s (excess flow valves fitted) ▪ Assume less than 0.1 kg released (both cases) 70 MPa ▪ 6 mm ID for cars; 11 mm ID for buses ▪ Isolation within 2 s (excess flow valve fitted) ▪ Assume less than 0.15 kg released (both cases)
S1	Rupture of CGH2 buffer storage output line, (e.g. underground line from CGH2 storage or cascade priority panel to dispenser)	Jet fire & explosion	YES	YES	▪ Pipe internal diameter ▪ Time for isolation (mitigated scenario) ▪ Inventory to be released	▪ 13 mm ID ▪ Assume contents of line is lost 35 MPa (max WP 43.8 MPa) Length of line 20 – 75 m 0.25 kg H2 for a 20 m U/G line 70 MPa (max WP 87.5 MPa) Length of line 20 – 75 m 0.4 kg H2 for a 20 m U/G line
S8	Burst of CGH2 hydrogen storage tank,	Burst (overpressure) & missiles	Not applicable	Not applicable	▪ Pressure vessel volume	Options could be: ▪ 50L standard industrial cylinder

Ref	Description	Phenomena	Non mitigated	Mitigated	Necessary data	Input from Industry
						▪ 90 L composite cylinder ▪ 6 m pressure vessel ▪ 10 m pressure vessel (worst case) 0.767 m^3 e.g., ASME
PR1	Steam reformer: Rupture of NG feed line inside production container,	Explosion	Not applicable	Not applicable	▪ NG pressure ▪ NG line internal diameter ▪ Volume of hydrogen production casing	- Pressure for compressor inlet / outlet: 2.3 / 16.0 barg - Line id for compressor inlet / outlet: approx. 20 / 12 mm - Volume of hydrogen production casing: 135 m3
T1	CGH2 trucked-in trailer hose disconnection during discharge (200 – 250 bar)	Jet fire & explosion	YES	YES	▪ Hose internal diameter / flow restriction ▪ Time for isolation (mitigated scenario) ▪ Inventory to be released	▪ Hose ID: 12.5 mm ▪ Assume all contents lost ▪ 250 kg H2 released
DL8	LH2 dispenser: Shear of the hose line,	Fire & explosion	YES	YES	▪ Hose internal diameter ▪ Pressure ▪ Time for isolation (mitigated scenario) ▪ Inventory to be released	▪ 7 – 8 mm hose ID ▪ Pressure: 3 – 8 bar ▪ Isolation: within 5 s ▪ Contents: 0.16 kg LH2
TL1	LH2 tanker discharge hose: Leakage after discharge when decoupling (hydrogen source not isolated),	Fire & explosion	YES	YES	▪ Hose internal diameter / flow restriction ▪ Pressure ▪ Time for isolation (mitigated scenario) ▪ Inventory to be released	▪ Hose ID: 22.5 mm ▪ Max WP pressure: 11 bar ▪ 4 min ▪ 100 kg LH2 estimated
SL3	LH2 Below ground storage failure (with vault),	Fire & explosion	YES	YES	▪ Vault dimensions ▪ Leak orifice ▪ Inventory to be released	▪ exposed vault area is: 4.6 m depth x 5.6 m width x 10.4 m long ▪ Orifice of 0.2 mm id

Ref	Description	Phenomena	Non mitigated	Mitigated	Necessary data	Input from Industry
						▪ 100 L of LH2 released
D6	CGH2 (35 & 70 MPa) Leakage at nozzle during refuelling,	Explosion & standing flame	NO	YES	▪ Leak equivalent orifice	Minor leakage: 0.10 mm ID Major leakage: 0.20 mm ID
D5	CGH2 (35 & 70 MPa) Hole in dispensing line	Explosion & standing flame	NO	YES	▪ Leak orifice	Minor leakage: 0.10 mm ID Major leakage: 0.20 mm ID
D3	CGH2 (35 & 70 Mpa) Leakage inside dispenser enclosure	Explosion	Not relevant	Not relevant	▪ Volume of dispenser enclosure	1.5 H x 1.0 L x 0.6 W (NB: cabinets are ventilated)
DL1	LH2 Leakage at nozzle during refuelling (12 Bar max WP)	Explosion	NO	YES	▪ Leak equivalent orifice	Minor leakage: 0.10 mm ID Major leakage: 0.20 mm ID
DL10	LH2: Hole in dispensing line	Explosion	NO	YES	▪ Leak orifice	Minor leakage: 0.10 mm ID Major leakage: 0.20 mm ID
S7	CGH2 Release of hydrogen through vent line	Explosion & jet fire	Not relevant	Not relevant	▪ Vent orifice ▪ Inventory to be released	▪ 12.5 mm ID orifice leading to a 25 mm ID vent line with discharge at least 3 m high above ground level ▪ Assume worst case release from a PV buffer cylinder; 25 kg H2 at 420 bar
SL1	LH2 Release of hydrogen through vent line (loss of vacuum)	Explosion & jet fire	Not relevant	Not relevant	▪ Vent orifice ▪ Inventory to be released	▪ 17 mm ID orifice leading to a 50 mm ID vent line with discharge at least 8 m above ground level; (discharge is as gaseous phase) ▪ Assume LH2 tank pressure of 10 bar; ▪worst case is 3,300 kg of LH2 (e.g., BP’s u/g LH2 tank) ▪expected case; assume 50 kgs LH2 (1 kg LH2 = 850 L GH2)

3 Selection of cases for simulation. Partition of modelling work

An event sequence of any accident scenario includes a number of individual phenomena. For example, a typical scenario of accident with hydrogen can include the following chain of events: formation of a source of H_2, mixing with air and formation of flammable mixture (a cloud or a volume filled with mixture), ignition of such mixture, combustion, flame acceleration, fast deflagration, deflagration-to-detonation transition, and detonation.

For successful simulation of such sequence of events a variety of modern numerical tools with highly qualified personnel is required.

3.1 Simulation capacities of project partners

The partners of the project have a number of specialized codes targeted to simulation of different stages in development of accident. Table 4 summarises an availability of the numerical tools both multi-dimensional CFD and simplified (integral) together with partners' expertise in the area of industrial safety.

Table 4 Numerical tools available for simulations from project partners

Partner	**Code**	**CFD/integral/other**	**Applicability area**
CEA	CAST3M	CFD	Dispersion & combustion (deflagration, detonation)
	SPHERE-1D	Simplified 1D spherical combustion	Combustion (deflagration, detonation)
	FLUENT	CFD	Dispersion
FZK	GASFLOW	CFD	Distribution/mixing mitigation devices
	COM3D, FLAME3D, DET3D		Combustion at different regimes, detonation, combustion mitigation
INERIS	PHOENICS, ARIARISK	CFD	Release, mixing and distribution
NCSRD	ADREA-HF	CFD	Release, mixing and distribution mitigation (venting, water spraying)
	GAJET	Integral	Discharge from CGH2 system
JRC	REACFLOW	CFD	Combustion combustion mitigation
ET	FLUENT, KAMELEON Fire-EX	CFD	Diffusion/mixing Combustion; mitigation

Examination of the probable scenarios shows that in the course of development of all of them the explosion processes can occur. To separate scenarios depending on expected hazard and possible damages one can distinguish 3 groups of scenarios:

- scenarios with small H_2 inventory: mass of $H_2 < 1$ kg (D4, S1, S8, DL8)
- scenarios with medium H_2 inventory: mass of $H_2 = 25 – 100$ kg (PR1, T1, TL1, S7, SL1)
- scenarios with large H_2 inventory: mass of $H_2 > 100$ kg (T1, SL1).

Of course, not all of them have the same hazard potential; however for the exhaustive Risk Assessment (RA) the data on combustion and explosion processes for all these cases should be available.

3.2 Share of simulation efforts

As it was already mentioned only 15 cases were planned for simulation. To obtain representative results, partners agreed to perform simulation of the scenarios for each of three groups. It was decided not to consider the effects of different surroundings (city, free field, motorway), which were foreseen initially, for the sake of higher coverage of scenario variations.

In summer 2006 the results of the tests on prototypical refuelling station performed by Shell Hydrogen B.V. and HSL were published. To increase reliability and trustworthiness of the predictions of simulations, it was decided broadly perform simulation of one of the cited experiments, with the aim to demonstrate abilities of the partners codes to achieve high reproducibility of experimental results and therefore their ability to predict development of considered accidents. The partners agreed to replace original scenario D4 by one of the referred tests. Here and below this test will be referenced as D4. Details on initial and boundary conditions can be found in Section 4.1.

In Table 5 a work share between partners is summarized. ET, CEA and FZK plan to model D4 scenario, which corresponds to one of jet release HSL - Shell experiments. NCSRD and JRC concentrated on scenarios with participation of liquid hydrogen: DL8 and TL1. ET and FZK are also planning to consider large-scale accident (250 kg of H_2) scenario T1. CEA additionally will consider scenarios S8 and PR1 using their integral (non-CFD) tools.

In the last column ‘Modelling work’ showing which cases which partner will simulate, the following notations and abbreviations are used:

- Leading D or C followed by semicolon is used to distinguish ‘Dispersion’ simulation from ‘Combustion’;
- Letter M means ‘mitigated’ case;
- m – ‘non-mitigated’ case;
- W – case with wind;
- w – case without wind;
- 350 – case with 35 MPa pressure;
- 700 – case with 70 MPa pressure.

Table 5- Project partners participation in the simulations for different scenarios

Ref	Description	External safety	Customer safety	Other	Mark	Phenomena	Non mitigated	Mitigated	Refuelling station class	Remarks	Wind effect	Proposed tool	Modelling work*
D4	Rupture of dispensing line (flexible hose),	▨			36	Dispersion & Explosion	YES (70 MPa)	YES (35 MPa)	Compressed 350 and 700 bar	Mitigation shall reduce release duration and quantity	YES, 5 m/s	CFD	D: ET (M, n, W, w, 350, 700) D : CEA (M, m, W, 350, 700) D : FZK (M, m, w, 350, 700) C : CEA (M, m, W) C : FZK (M, m, w, pre-mixed)
						Jet Fire	YES	Not necessary			No	“Basic” calculation spread sheet / 1D model	-
S8	Burst of hydrogen storage tank,	▨			54	Burst (overpressure) & missiles	Not applicable	Not applicable	Compressed 700 bar	Burst of one tank. Effect of protection wall to be considered.	No	“Basic” calculation spread sheet / 1D model	C: CEA (non-CFD)
PR1	Rupture of NG feed line inside production container	▨			36	Explosion	Not applicable	Not applicable	Compressed	Explosive atmosphere inside container.	Not relevant	“Basic” calculation spread sheet / 1D model	C: CEA (non-CFD)

Ref	Description	External safety	Customer safety	Other	Mark	Phenomena	Non mitigated	Mitigated	Refuelling station class	Remarks	Wind effect	Proposed tool	Modelling work*
T1	Trailer hose disconnection during refilling	▨			54	Dispersion & Explosion	YES	YES	Compressed 250 bar	Is likely to be more severe than D4. Mitigation shall reduce release duration and quantity	YES, 5 m/s	CFD	D: ET (M, m, W, w) D: FZK (m, w) C: FZK (m, w)
						Jet Fire	YES	Not necessary			No	“Basic” calculation spread sheet / 1D model	-
DL8	Shear of the hose line,	▨			36	Dispersion & Explosion	YES	YES	Liquid 8 bar	Mitigation shall reduce release duration and quantity	YES, 5 m/s	CFD	D: NCSRD (M, m, W, w) C: JRC (M, m, W, w)
						Pool fire	YES	YES			No	1D model for heat loads	-
TL1	Tanker dispensing line disconnection during refuelling	▨			54	Dispersion & Explosion	YES	YES	Liquid 11 bar	Is likely to be more severe than DL8. Mitigation shall reduce release duration and quantity	YES, 5 m/s	CFD	D: NCSRD (M, m, W, w) C:JRC (M, m, W, w)
						Pool fire	YES	YES			No	1D model for heat loads	-

4 Initial and boundary conditions. Specification of Refuelling Station layout

The choice of geometrical environment for simulation of the explosion process is of major importance, as it can often establish the character of the explosion, its strength and possible consequences. At the beginning of the simulations the generic Refuelling Station (RS) layout (which has to be developed in WP1) was not finalized, it was decided to use model layouts based on the following prototypes:

- For simulations of scenarios D4 and DL8, the layout of Shell - HSL jet release experiments;
- For simulations of scenarios T1 and TL1, the layout based on Washington DC refuelling station storage / transport area;
- For simulations of scenarios S8 and PR1, there is no need in surroundings details due to 1D (0D) character of calculations – no layout assumptions.

4.1 Cases D4 and DL8

In the experiments[2] initiated by Shell, aimed to study hazard potential associated with deflagration of high-pressure leaks from hydrogen vehicle refuelling systems, the conditions, which were very close to those of scenarios with dispenser failure, were used.

Quoting the referred work[2]: "In this case study, the main components of a refuelling station were reproduced, albeit in a simplified and robust form. The refuelling station was represented by a dummy vehicle and two dispensers. A confining wall was also used to represent either a large vehicle alongside the dispensers or an actual wall. The need for a canopy over the refuelling station was rejected because it would not significantly alter the development of a deflagration among the congestion within 2.5 m of the ground."

Thus, the possibility to use experimental data for additional validations of dispersion and combustion simulations, from one side, and clearness and simplicity (what is important also for interpretation of simulation results), from other side, determined our choice of RS layout in favour of Shell / HSL test site.

The referred study included two types of experiments: premixed and jet release experiments. In the first type the configuration (Figure 1) was fitted within a region 5.4 m x 6.0 m x 2.5 m (high) delineated by a frame covered in a thin plastic film so that the components could be enveloped in a homogeneous hydrogen–air clouds to determine the 'worst-case' deflagration overpressures. The mixture concentration chosen was optimal to generate the highest overpressure.

In the second type the configuration (Figure 2) was almost the same: the frame was removed and the dispensers were slightly dislocated (order of 10 cm). The changes in

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[2] L C Shirvill and T A Roberts, 2006, Designing for Safe Operations: Understanding the Hazards Posed by High-Pressure Leaks from Hydrogen Vehicle Refuelling Systems, National Hydrogen Association Annual Hydrogen Conference, March 12-16, 2006.

layout details were accepted to be negligible, therefore further we will not distinguish between them.

Figure 1 View of refuelling station model used in premixed experiments. Plastic film covering the frame is not shown

Figure 2 View of refuelling station model used in jet release experiments. Comparison with real car

4.1.1 Geometry

Dispensers. The two simulated hydrogen dispensers were 0.6 m x 0.9 m x 2.1 m high steel boxes that were flanged at the bottom so that they could be bolted to the concrete pad. The internal volume of each dispenser was ca. 1.07 m^3 and the external volume ca. 1.13 m^3.

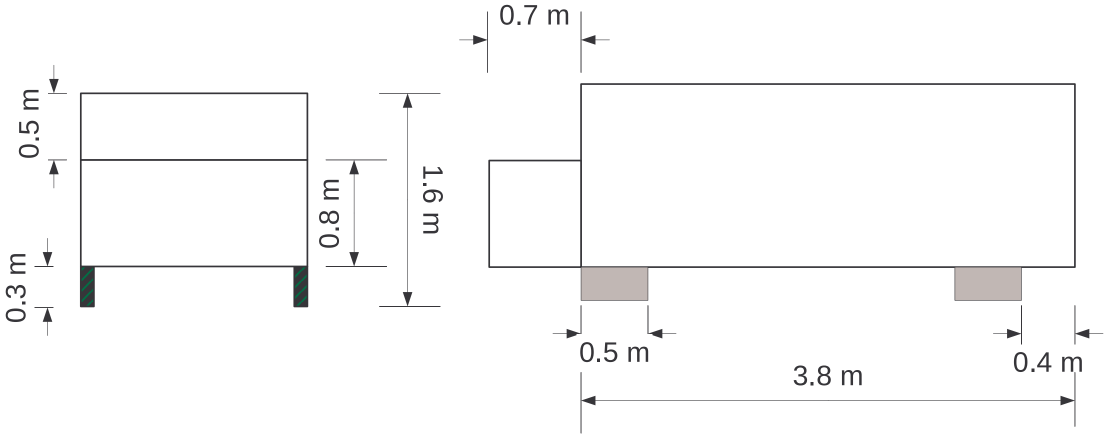


Figure 3 Model of vehicle used in experiments

Figure 4 Model of vehicle for simulations

Vehicle. The vehicle was fabricated from a framework of 100 x 100 x 8 mm square hollow section (SHS) steel. This was clad in 6 mm thick mild steel in the sides and top of the “passenger” section (1.7 m wide, 1.3 m high and 3.8 m long) and 8 mm thick plate for the “engine bay” section (1.7 m wide, 0.8 m high and 0.7 m long) and the bottom of the “passenger” section. The “passenger” section was sealed at the bottom (i.e. no gas could get in) and reinforced with SHS cross members. The “engine bay” section left open at the bottom so it could fill with gas. Two lengths of SHS braced the end of the “engine bay” against the top of the “passenger compartment. The welded assembly was raised 0.3 m off the ground by 0.3 m high supports made from two 0.1 m steel box sections welded to L-section representing wheels. The vehicle was bolted to the concrete pad through the outer part of each L-section. The total volume (i.e. the volume where no hydrogen can enter) of the vehicle was 8.56 m^3. A diagram of the vehicle for simulations is shown in Figure 4.

Wall. The 4.8 m high, 5.4 m long wall is constructed from 0.60 x 0.60 x 1.80 m concrete blocks.

Frame. The refuelling rig is surrounded by a 5.4 x 6.0 x 2.5 m frame made from 25 mm square hollow section steel. The frame was butted up against the wall. In the series of premixed experiments the frame and the outside of the wall were covered with a thin (23 µm) plastic film, similar to cling film. The film was held to the sides of the frame by using spray-on contact adhesive. The gap between the bottom of the frame and the concrete pad was filled with expanding polyurethane foam to minimise gas leakage.

4.1.2 Hydrogen source and ignition location

Details of hydrogen injection are shown in Figure 5 and Figure 8. In Figure 8 the location of H_2 injection is designated with marker ‘R1’. It is located in the middle between dispenser and vehicle.

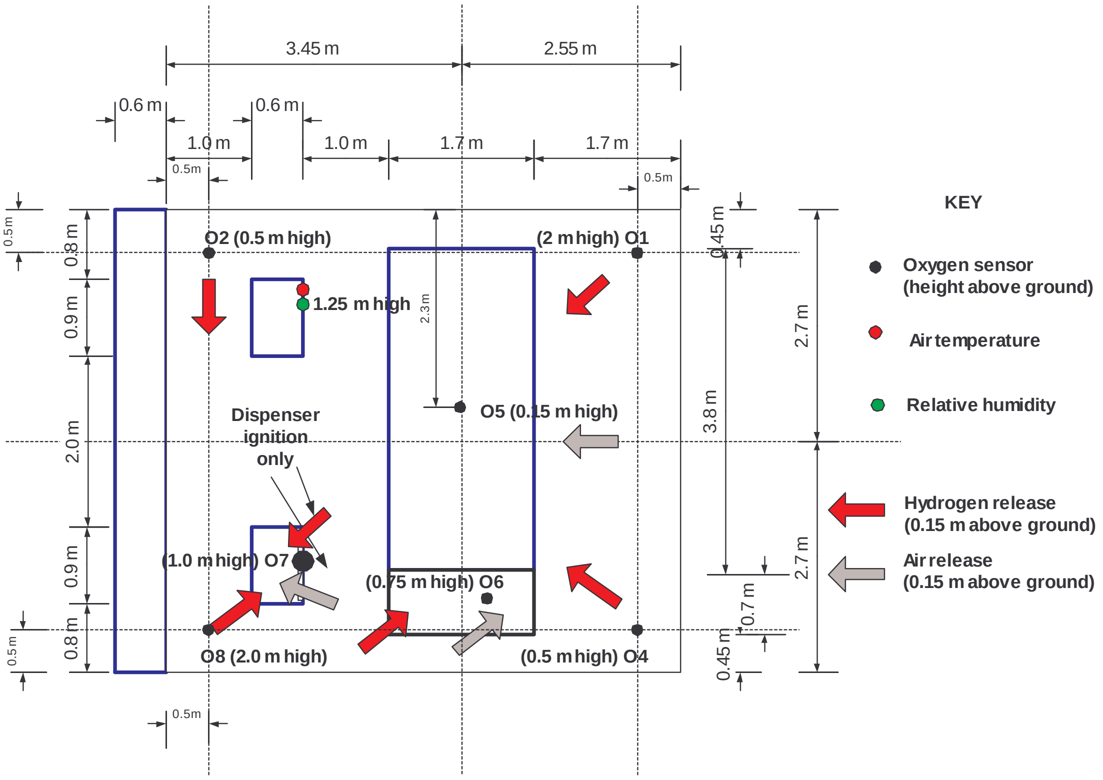


Figure 5 Fuel and air outlet positions and gas sensor positions

The time history of pressure (PVVP2) in the vessel imitating dispenser and temperature at dispenser nozzle (TPVT5) are presented in Figure 6.

Taking into account the differences between real experimental conditions and theoretically expected ones (listed in Table 3) we have corrected leakage data for scenario D4, which were accepted as being reproduced in the experiment:

- source 600 g of hydrogen during 0.7 s, temperature –20 °C at nozzle by 35 MPa inside (mitigated case);
- source mass flow rate 100 g/s of hydrogen during 2 s, temperature at nozzle –20 °C by 70 MPa inside (mitigated case);
- source mass flow rate source 100 g/s permanently, temperature at nozzle –20 °C by 70 MPa inside (non-mitigated case);

- source mass flow rate source 100 g/s permanently, temperature at nozzle –20 °C by 35 MPa inside (non-mitigated case).

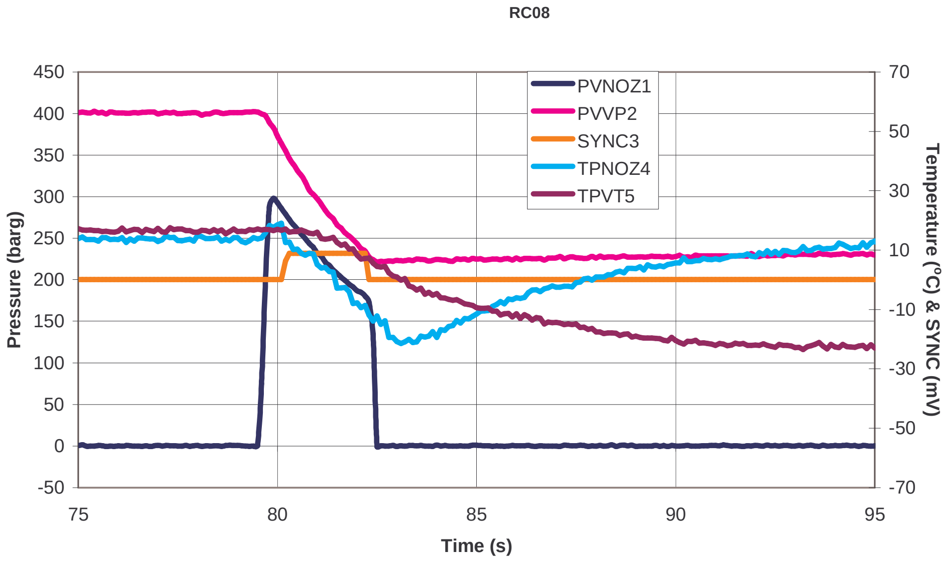
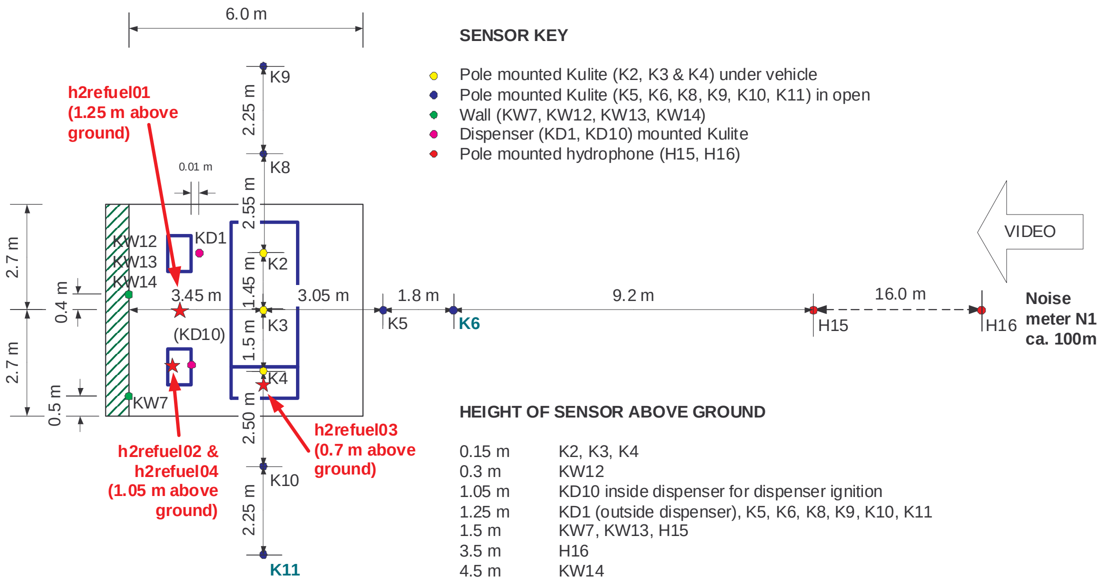


Figure 6 Pressure and temperature transducers recording in jet release experiments

4.1.3 *Transducers locations*

In Figure 7 and Figure 8 the positions of transducers and location of ignition point are shown. Figure 7 illustrates the layout of premixed trials. Ignition point in these tests is located on middle line between dispensers. It corresponds to location ‘S3’ in Figure 8.



0.15 m	K2, K3, K4
0.3 m	KW12
1.05 m	KD10 inside dispenser for dispenser ignition
1.25 m	KD1 (outside dispenser), K5, K6, K8, K9, K10, K11
1.5 m	KW7, KW13, H15
3.5 m	H16
4.5 m	KW14

Figure 7 Pressure sensor and ignition positions for premixed trials

Figure 8 outlines the arrangement of jet release experiments. Ignition point in these trials is located underneath the ‘engine bay’ of the model vehicle and is designated with symbol ‘S2’.

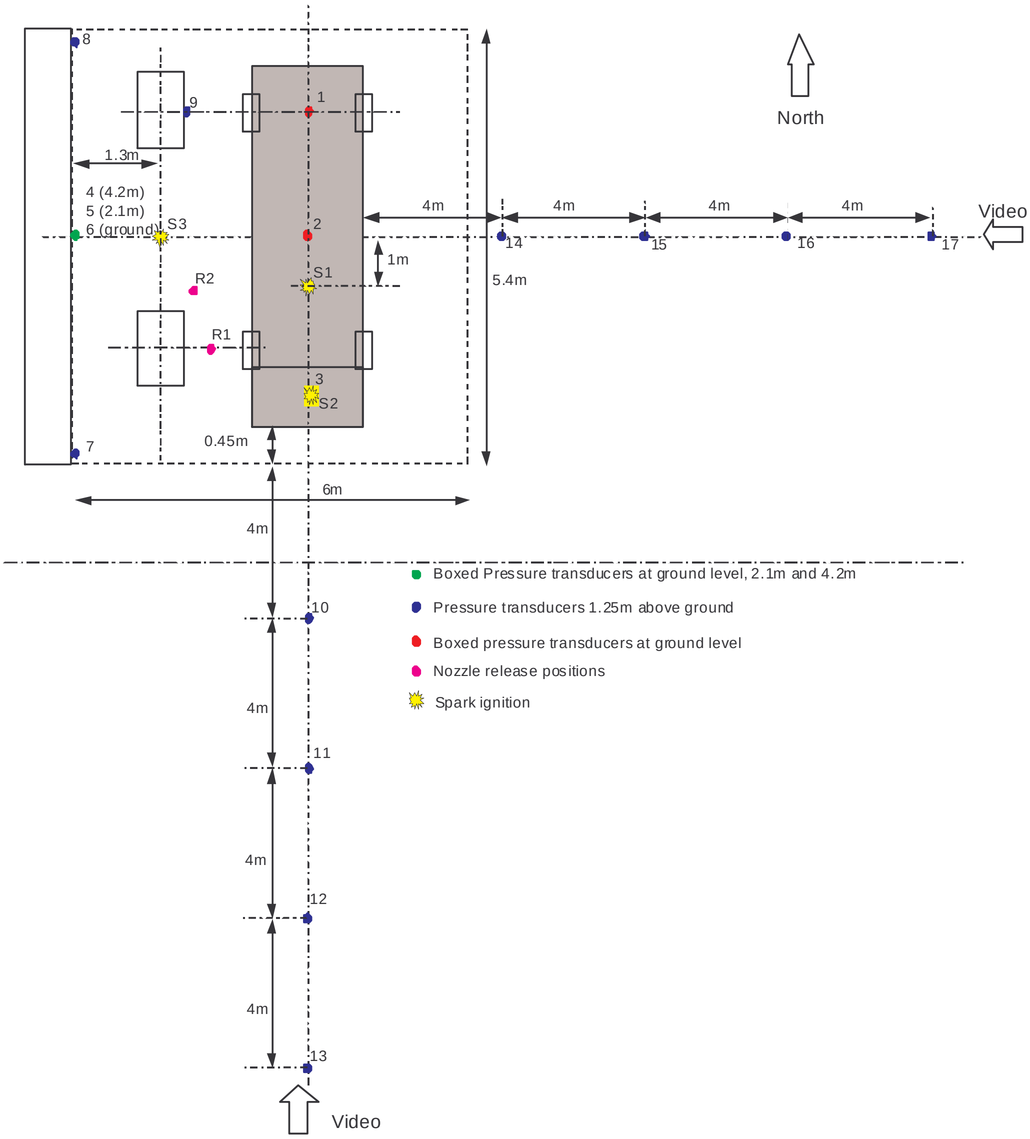


Figure 8 Pressure sensor and ignition positions for jet release trials

4.2 Cases T1 and TL1

The layout of storage / transport area of RS taken as prototypical for simulation of scenarios T1 and TL1 is based on the Hydrogen Refuelling Station (HRS) situated at Washington DC. This layout was chosen because it exhibits all characteristic features of known RSs and the geometrical data (dimensions, equipment, layout, even drawings, etc.) were made available to the partners in the HyApproval project.

In Figure 9 and Figure 10, sketches showing all important equipment with their mutual arrangement for a liquid H_2 refuelling station are given. This layout will be used for the simulation of the TL1 case and is based on the HRS situated at Washington DC.

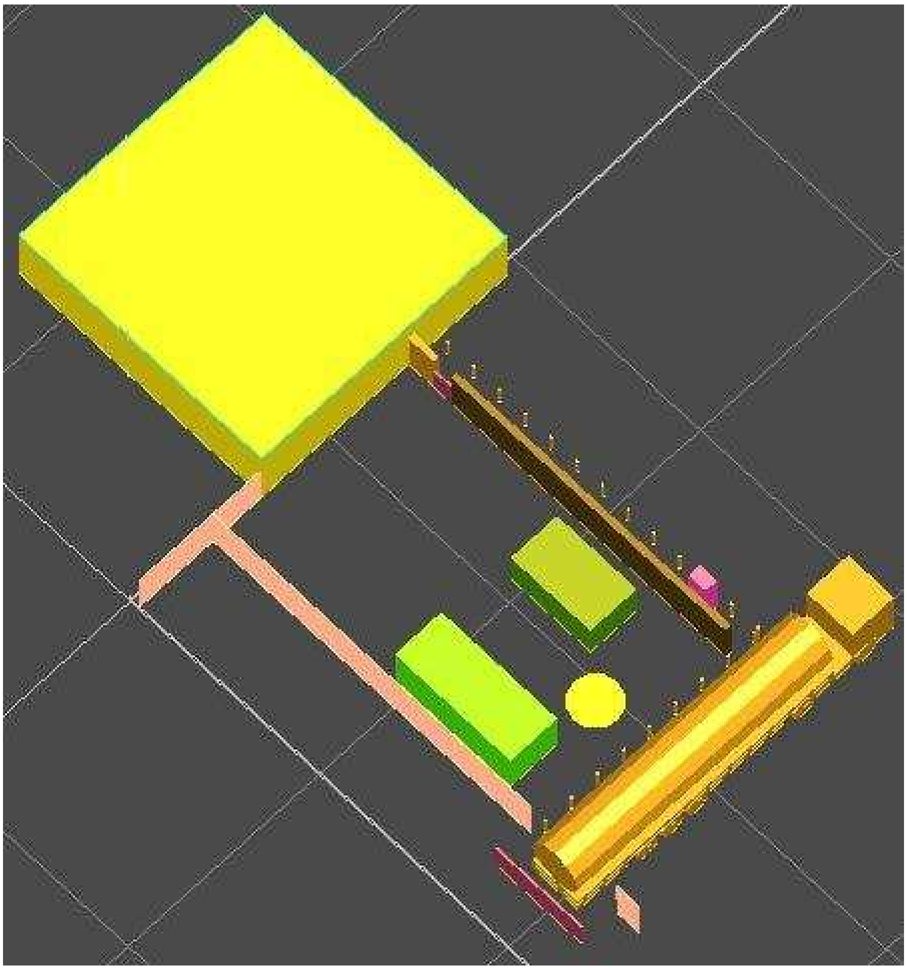


Figure 9 LH2 Refuelling Station Ground View (based on Washington HRS)

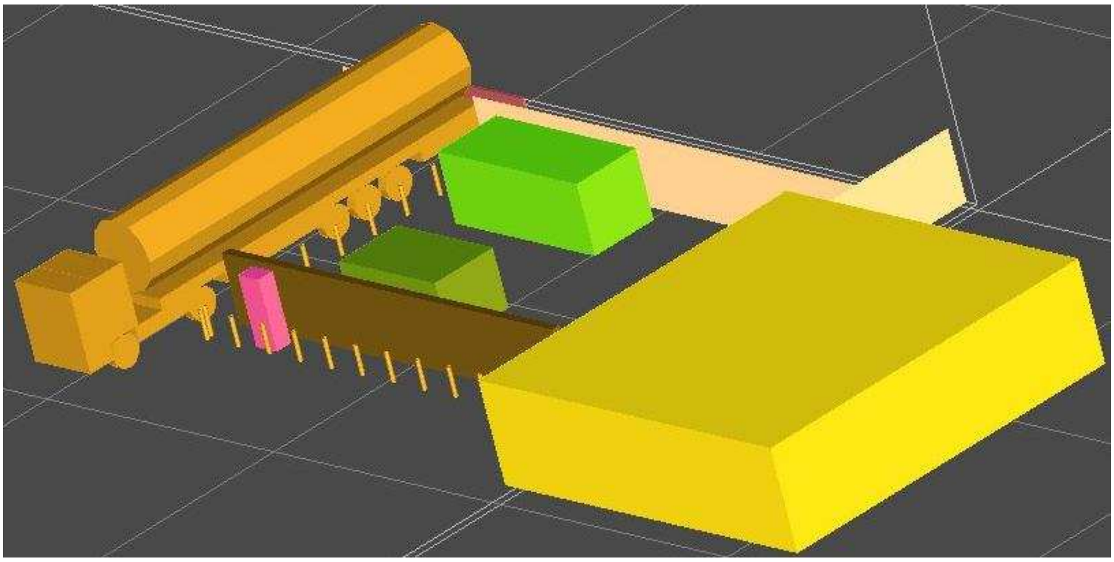


Figure 10 LH2 Refuelling Station Side View

The following table, **Fehler! Verweisquelle konnte nicht gefunden werden.**, shows the geometrical data of the liquid H_2 refuelling station. The equipments are presented as boxes and cylinders. The coordinates of the lower left corner and the size of each box are given while for each cylinder the coordinates of its centre and the diameter and size are given.

Table 6 LH2 Refuelling Station Geometrical Data

		Position of the lower left corner			**Size**		
		X (mm)	**Y (mm)**	**Z (mm)**	**X (mm)**	**Y (mm)**	**Z (mm)**
1	Existing building	-12388.0	6388.0	0.0	12888.0	12888.0	3500.0
2	Storage tube	9464.0	10602.0	100.0	4232.0	2438.0	2000.0
3	Compressor tube	9352.0	4612.0	100.0	6156.0	2462.0	2400.0
4	Concrete wall (part 1)	500.0	14093.0	0.0	1346.0	300.0	2400.0
5	Concrete wall (part 2)	2760.0	14093.0	0.0	14572.0	300.0	2400.0
6	Dispenser	14748.0	14705.0	0.0	900.0	600.0	2400.0
7	Fence 1	450.0	0.0	0.0	50.0	6388.0	2438.0
8	Fence 2	500.0	3838.0	0.0	16832.0	50.0	2438.0
9	Parts of LH2 truck-trailer	18618.5	18300.5	512.0	2438.0	964.5	2683.0
10		18618.5	17080.0	1081.0	2438.0	1220.5	2114.0
11		18618.5	14540.5	577.0	2438.0	2679.0	504.0
12		18618.5	2665	1081.0	2438.0	13410.0	371.0
13		18618.5	8940.5	706.0	2438.0	4519.0	375.0
14		18618.5	7640.5	706.0	2438.0	219.0	375.0
15		18618.5	6340.5	706.0	2438.0	219.0	375.0
16		18618.5	2665.0	706.0	2438.0	2594.5	375.0
17	Sliding gate	17349.0	2000.0	0.0	4572.0	100.0	1500.0
18	Gate	1846.0	14093.0	0.0	914.0	100.0	1500.0
19	Fence 3	21921.0	3838.0	0.0	1154.0	50.0	2438.0
		Position of centre			Diameter	Length	
20	H2 tank	15203.0	9370.0	37.5	2272.0	75.0	
21	Bollards	1200.0	15468.0	500.0	150.0	1000.0	
22		2569.0	15468.0	500.0	150.0	1000.0	
23		3938.0	15468.0	500.0	150.0	1000.0	
24		5307.0	15468.0	500.0	150.0	1000.0	
25		6676.0	15468.0	500.0	150.0	1000.0	
26		8045.0	15468.0	500.0	150.0	1000.0	
27		9414.0	15468.0	500.0	150.0	1000.0	
28		10783.0	15468.0	500.0	150.0	1000.0	
29		12152.0	15468.0	500.0	150.0	1000.0	
30		13521.0	15468.0	500.0	150.0	1000.0	
31		14890.0	15468.0	500.0	150.0	1000.0	
32		16259.0	15468.0	500.0	150.0	1000.0	
33		17628.0	15468.0	500.0	150.0	1000.0	
34		17679.0	15250.0	500.0	150.0	1000.0	
35		17679.0	13881.0	500.0	150.0	1000.0	
36		17679.0	12512.0	500.0	150.0	1000.0	
37		17679.0	11143.0	500.0	150.0	1000.0	
38		17679.0	9774.0	500.0	150.0	1000.0	
39		17679.0	8405.0	500.0	150.0	1000.0	
40		17679.0	7036.0	500.0	150.0	1000.0	
41		17679.0	5667.0	500.0	150.0	1000.0	

42		17679.0	4298.0	500.0	150.0	1000.0
43	Parts of LH2 truck-trailer	19837.5	9370.0	2671.0	2438.0	13410.0
44		18787.5	17760.0	540.5	1081.0	338.0
45		20887.5	17760.0	540.5	1081.0	338.0
46		18787.5	14000.0	540.5	1081.0	338.0
47		20887.5	14000.0	540.5	1081.0	338.0
48		18787.5	8400.0	540.5	1081.0	338.0
49		20887.5	8400.0	540.5	1081.0	338.0
50		18787.5	7100.0	540.5	1081.0	338.0
51		20887.5	7100.0	540.5	1081.0	338.0
52		18787.5	5800.0	540.5	1081.0	338.0
53		20887.5	5800.0	540.5	1081.0	338.0

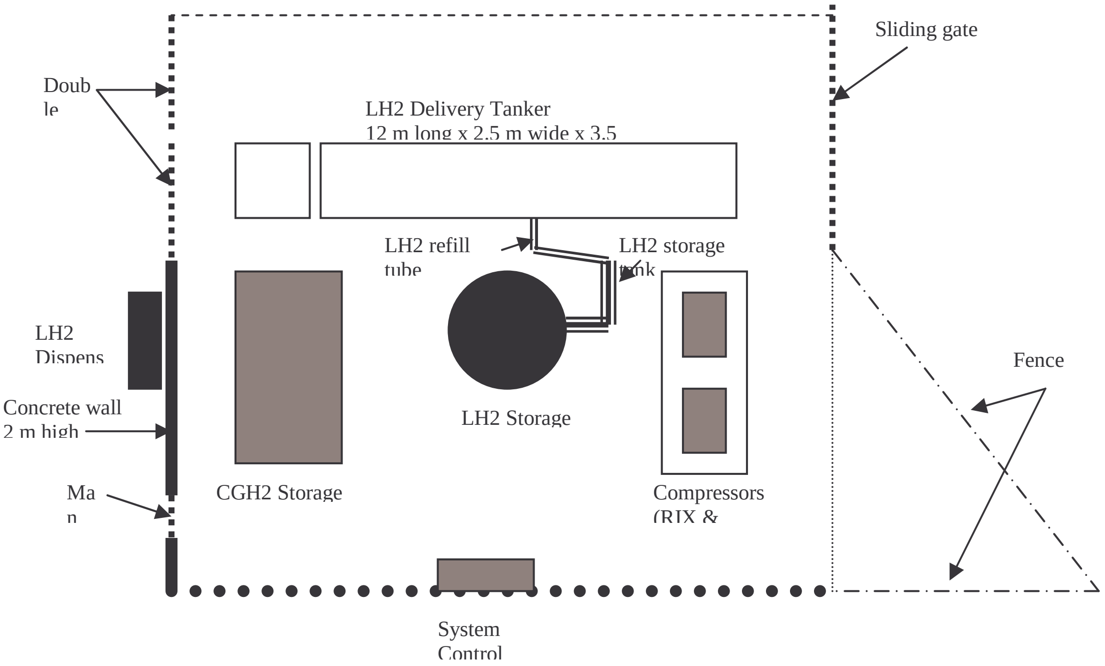


Figure 11 Sketch of simplified layout for liquid hydrogen storage / transport area based on Washington HRS

In Figure 12, a sketch showing all important equipment with their mutual arrangement for gas H_2 refuelling station is placed. This layout will be used for the simulation of the T1 case and it is based on the H_2 refuelling station at Luxembourg.
Fehler! Verweisquelle konnte nicht gefunden werden. shows the geometrical data of the CGH_2 refuelling station main components. Again, each component is represented as box or cylinder.
Fehler! Verweisquelle konnte nicht gefunden werden. shows the geometrical data of the lean-to roofs for weather protection of the CGH_2 station. Two lean-to roofs exist in the layout, one for the buffer storage and one for the compressor module. Each roof consists of two parts with two surfaces each. In **Fehler! Verweisquelle konnte nicht gefunden werden.** the coordinates of the 4 points of each surface are presented.

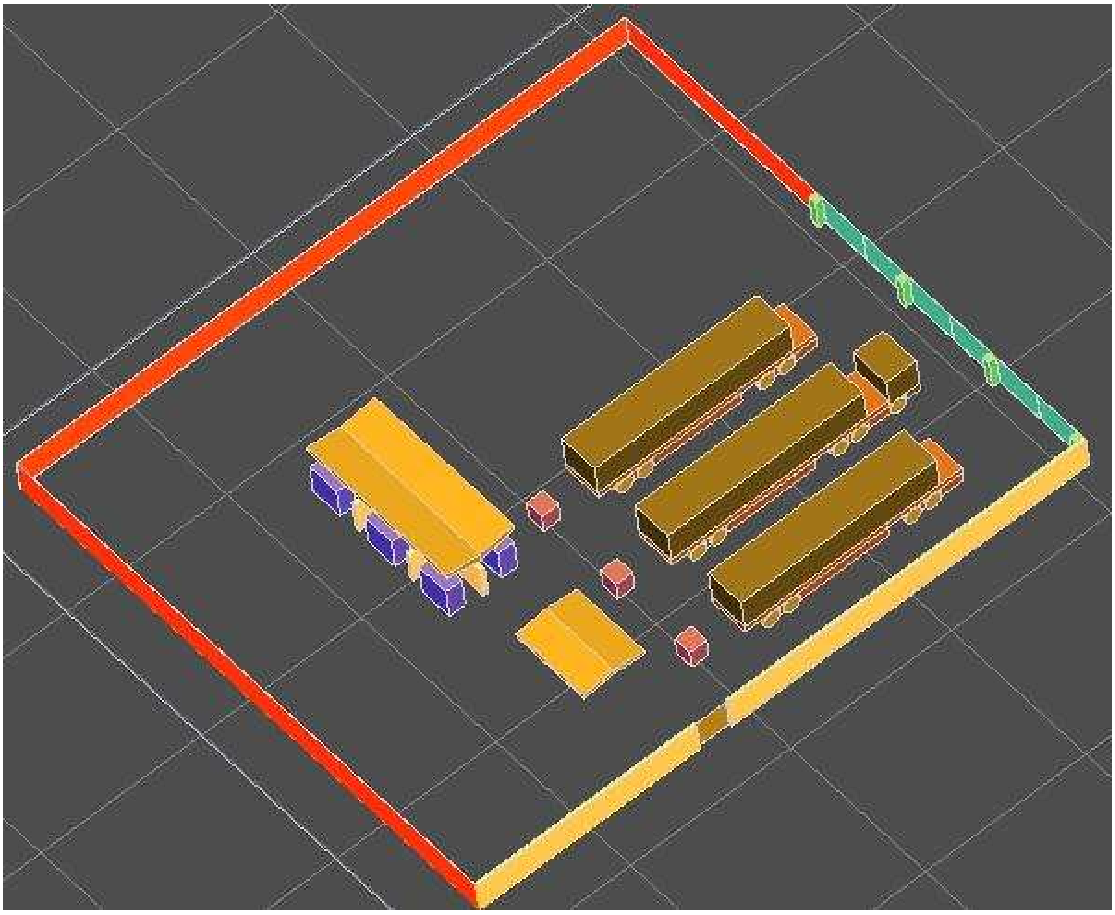


Figure 12 CGH2 Refuelling Station Side View (Luxembourg refuelling station)

Table 7 CGH2 Refuelling Station Geometrical Data (main components)

		Position of lower left corner			Size		
		X (mm)	Y (mm)	Z (mm)	X (mm)	Y (mm)	Z (mm)
1	Buffer storage bundle 1	12830	16290	0.0	2000	1000	2000
2	Buffer storage bundle 2	16910	16290	0.0	2000	1000	2000
3	Buffer storage bundle 3	20940	16290	0.0	2000	1000	2000
4	Buffer storage bundle 4	12830	13040	0.0	2000	1000	2000
5	Buffer storage bundle 5	16910	13040	0.0	2000	1000	2000
6	Buffer storage bundle 6	20940	13040	0.0	2000	1000	2000
7	Buffer storage block wall 1	12830	14990	0.0	10330	300	2000
8	Buffer storage block wall 2	15830	15290	0.0	300	1850	2000
9	Buffer storage block wall 3	19860	15290	0.0	300	1850	2000
10	Buffer storage block wall 4	15830	13140	0.0	300	1850	2000
11	Buffer storage block wall 5	19860	13140	0.0	300	1850	2000
12	Compressor	28600	15200	0.0	2400	1000	1000
13	Unloading station 1	21460	19300	600	1130	1040	1200
14	Unloading station 2	26960	19300	600	1130	1040	1200
15	Unloading station 3	32460	19300	600	1130	1040	1200
16	Part of entrance gate 1	17170	40550	0.0	450	450	2000
17	Part of entrance gates 2&3	23630	40550	0.0	450	450	2000
18	Part of entrance gates 4&5	30090	40550	0.0	450	450	2000
19	Part of entrance gate 6	36550	40550	0.0	450	450	2000
20	Part 1 of concrete wall	37000	3000	0.0	200	13700	2000
21	Gate	37000	16700	0.0	15	2000	1800

22	Part 2 of concrete wall	37000	18700	0.0	200	22300	2000
23	Fence 1	3000	2985	0.0	34000	15	2000
24	Fence 2	2985	2985	0.0	15	38015	2000
25	Fence 3	3000	40985	0.0	14170	15	2000
26	Entrance gate 1	17620	41000	0.0	3005	15	2000
27	Entrance gate 2	20625	41000	0.0	3005	15	2000
28	Entrance gate 3	24080	41000	0.0	3005	15	2000
29	Entrance gate 4	27085	41000	0.0	3005	15	2000
30	Entrance gate 5	30540	41000	0.0	3005	15	2000
31	Entrance gate 6	33545	41000	0.0	3005	15	2000
32	Parts of trailer 1	20686	34512	380	2438	1374	620
33		20686	22320	1385	2438	12192	1975
34		20686	22320	1000	2438	13566	385
35		20686	25680	380	2438	5530	620
36		20686	33262	380	2438	250	620
37		20686	24430	380	2438	250	620
38	Parts of truck-trailer	26124	35886	1000	2438	1860	1860
39		26124	36886	500	2438	860	500
40		26124	34512	380	2438	1374	620
41		26124	22320	1385	2438	12192	1975
42		26124	22320	1000	2438	13566	385
43		26124	25680	380	2438	5530	620
44		26124	33262	380	2438	250	620
45		26124	24430	380	2438	250	620
46	Parts of trailer 2	31562	34512	380	2438	1374	620
47		31562	22320	1385	2438	12192	1975
48		31562	22320	1000	2438	13566	385
49		31562	25680	380	2438	5530	620
50		31562	33262	380	2438	250	620
51		31562	24430	380	2438	250	620

		Position of centre			Diameter	Length
52	Parts of trailer 1	20832.5	34012	500.0	1000	293
53		21125.5	34012	500.0	1000	293
54		22977.5	34012	500.0	1000	293
55		22684.5	34012	500.0	1000	293
56		20832.5	32762	500.0	1000	293
57		21125.5	32762	500.0	1000	293
58		22977.5	32762	500.0	1000	293
59		22684.5	32762	500.0	1000	293
60		20832.5	25180	500.0	1000	293
61		21125.5	25180	500.0	1000	293
62		22977.5	25180	500.0	1000	293
63		22684.5	25180	500.0	1000	293
64		20832.5	23930	500.0	1000	293
65		21125.5	23930	500.0	1000	293
66		22977.5	23930	500.0	1000	293
67		22684.5	23930	500.0	1000	293
68	Parts of truck-trailer	26270.5	36386	500.0	1000	293
69		26563.5	36386	500.0	1000	293
70		28415.5	36386	500.0	1000	293
71		28122.5	36386	500.0	1000	293

72		26270.5	34012	500.0	1000	293
73		26563.5	34012	500.0	1000	293
74		28415.5	34012	500.0	1000	293
75		28122.5	34012	500.0	1000	293
76		26270.5	32762	500.0	1000	293
77		26563.5	32762	500.0	1000	293
78		28415.5	32762	500.0	1000	293
79		28122.5	32762	500.0	1000	293
80		26270.5	25180	500.0	1000	293
81		26563.5	25180	500.0	1000	293
82		28415.5	25180	500.0	1000	293
83		28122.5	25180	500.0	1000	293
84		26270.5	23930	500.0	1000	293
85		26563.5	23930	500.0	1000	293
86		28415.5	23930	500.0	1000	293
87		28122.5	23930	500.0	1000	293
88	Parts of trailer 2	31708.5	34012	500.0	1000	293
89		32001.5	34012	500.0	1000	293
90		33853.5	34012	500.0	1000	293
91		33560.5	34012	500.0	1000	293
92		31708.5	32762	500.0	1000	293
93		32001.5	32762	500.0	1000	293
94		33853.5	32762	500.0	1000	293
95		33560.5	32762	500.0	1000	293
96		31708.5	25180	500.0	1000	293
97		32001.5	25180	500.0	1000	293
98		33853.5	25180	500.0	1000	293
99		33560.5	25180	500.0	1000	293
100		31708.5	23930	500.0	1000	293
101		32001.5	23930	500.0	1000	293
102		33853.5	23930	500.0	1000	293
103		33560.5	23930	500.0	1000	293

Table 8 CGH2 Refuelling Station Geometrical Data (with lean-to roofs for weather protection)

		X (mm)	Y (mm)	Z (mm)
1	Buffer storage Lean-to roof surface 1	12830	13040	3600
2		23160	13040	3600
3		23160	15140	3300
4		12830	15140	3300
5	Buffer storage Lean-to roof surface 2	12830	13040	3300
6		23160	13040	3300
7		23160	15140	2800
8		12830	15140	2800
9	Buffer storage Lean-to roof surface 3	12830	15140	3300
10		23160	15140	3300
11		23160	17290	3600
12		12830	17290	3600
13	Buffer storage Lean-to roof surface 4	12830	15140	2800

14		23160	15140	2800
15		23160	17290	3300
16		12830	17290	3300
17	Compressor Lean-to roof surface 1	27300	13800	2250
18		32300	13800	2250
19		32300	15700	2500
20		27300	15700	2500
21	Compressor Lean-to roof surface 2	27300	13800	2000
22		32300	13800	2000
23		32300	15700	2250
24		27300	15700	2250
25	Compressor Lean-to roof surface 3	27300	15700	2500
26		32300	15700	2500
27		32300	17600	2250
28		27300	17600	2250
29	Compressor Lean-to roof surface 4	27300	15700	2250
30		32300	15700	2250
31		32300	17600	2000
32		27300	17600	2000

4.2.1 Hydrogen source and ignition location

Since there are no indications on selection of the details of hydrogen source and ignition locations; their choice has to be performed taking into account general approach of safety simulations, namely the scenario followed by the worst case damages has to be taken for the consideration.

In Figures 13 and 14 the hydrogen source taken in simulations for scenario T1 is detailed. The coordinates are $x = 27.343$ m, $y = 22.32$ m and $z = 1.5$ m based on the geometry given in the Tables 7 and 8.

The direction of leaking hydrogen flow is horizontal (parallel to the y-axis), originates from the middle truck-trailer and faces the middle unloading station. Note that the 3 unloading stations were assumed to have a height of 1.9 m.

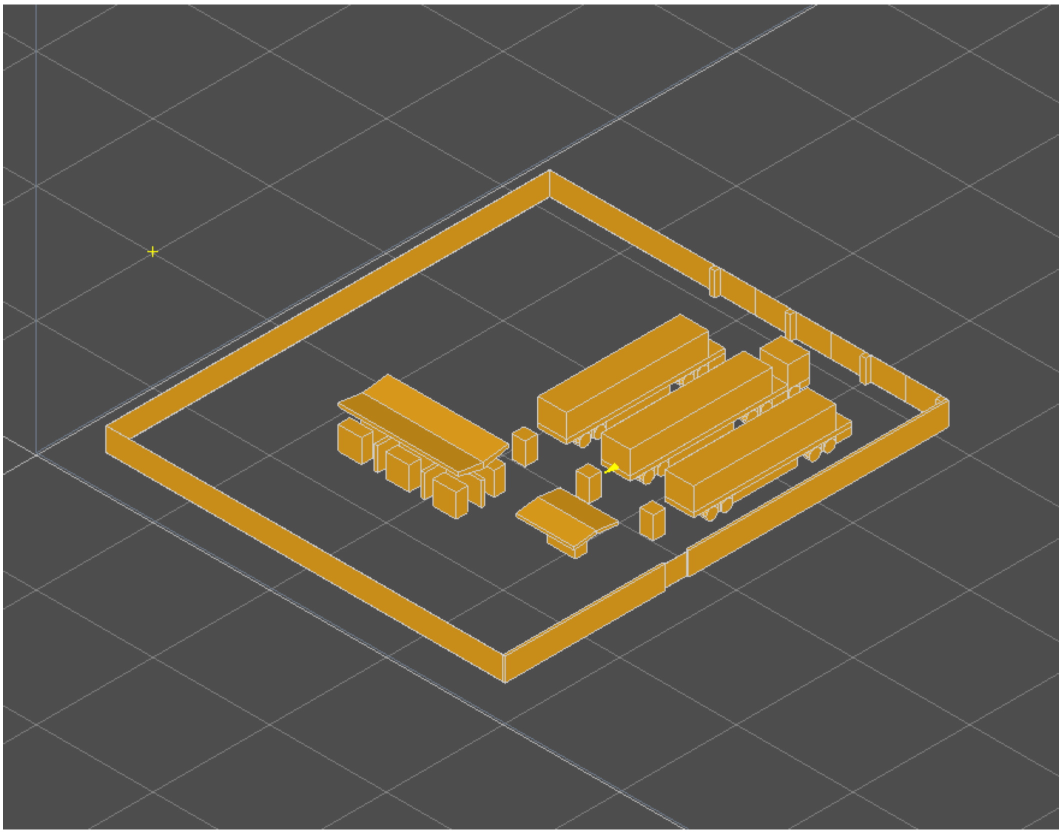


Figure 13 Location of leak for scenario T1. The leak originates from the middle truck-trailer and faces the middle unloading station

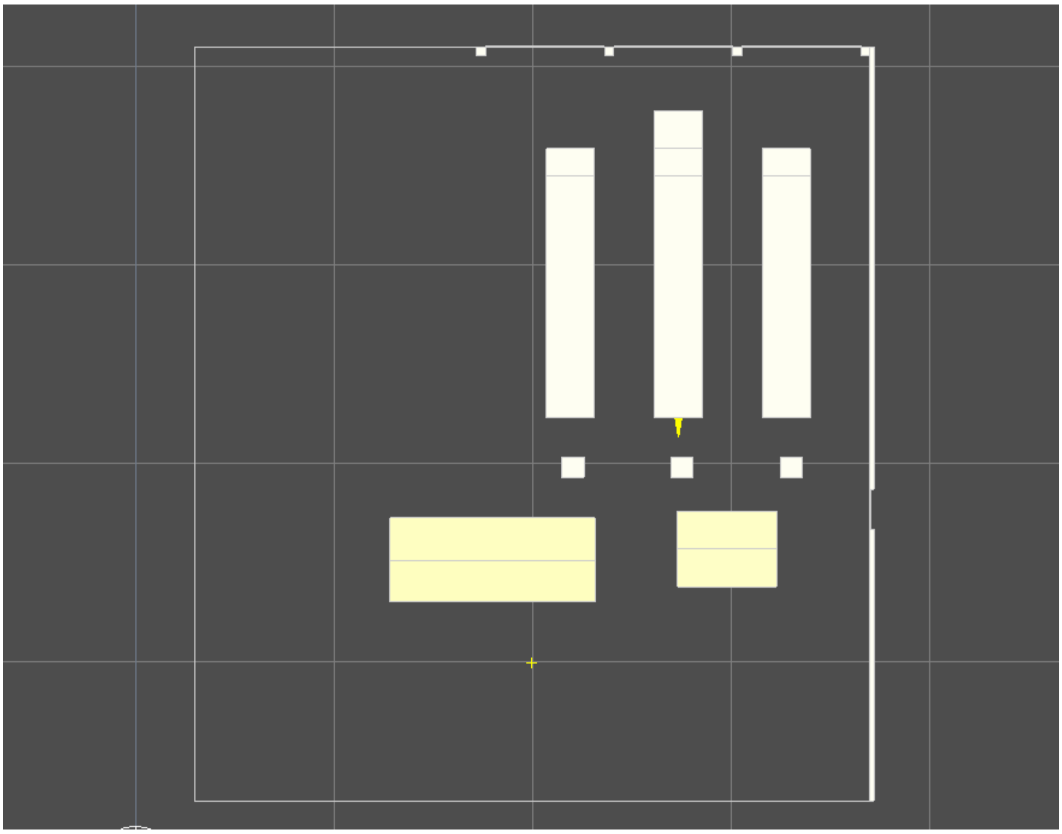


Figure 14 Location of leak for scenario T1. Top view

4.2.2 Transducers locations

The transducer locations were chosen so as to obtain information about the explosion-generated over-pressures at critical locations, such as

- the weakest equipment or constructions;
- the expected highest hazard potential; and
- to obtain information on how the blast loads decay with distance.

-

5 Validity of numerical tools

The adequacy of the numerical tools used in simulations is one of critical issues in computer modelling in general and in safety analysis in particular. All of the partners have performed systematic and thorough codes validation. Each of them has its own intensive programme of verification and validation activities. The validity issues themselves belongs to the special area of technical knowledge and are beyond the scope of this document (deliverable). However due to importance of this subject we have annexed a collection of papers devoted to different aspects of validation of the partners' codes.

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