Benefits of coupling FLACS-CFD® and LS-DYNA® for hydrogen safety applications

Pierre Glay[1], Laurent Paris[2]

[1]Dynamore France SAS, Versailles, France
[2]Gexcon France SARL, Paris, France

1 Introduction

1.1 Hydrogen in the global energy transition

There is a need for transitioning to an energy system with less greenhouse gas emissions and more sustainable energy production and consumption. A long-term structural change in energy systems is needed. Germany and France, among other countries, have decided to scale up the green hydrogen sector, with fundings of 9 billion and 7 billion euros respectively in the next 10 years.

Hydrogen as a new energy vector has many advantages over traditional hydrocarbon-based fuels. It is energy-efficient and can be environmentally friendly if it is be obtained from renewable sources. Potentially, in the future, it can solve many ecological and energy security issues. For more than a century, hydrogen has been produced and used for commercial and industrial purposes with a high safety record. However, the wider use of Fuel Cells and Hydrogen (FCH) technologies by the public (and not only by trained professionals) will require a new safety culture, innovative safety strategies, and breakthrough engineering solutions.

1.2 Hydrogen production and storage facilities

To meet the needs of public and private stakeholders involved in the development, construction, and operation of the hydrogen facilities needed to support the widespread roll-out of hydrogen fuel cell electric vehicles, modular station concepts including on-site production are the preferred technological solutions.

Hydrogen has a high energy content by weight, but not by volume, which is a particular challenge for storage. To store enough hydrogen gas, it's compressed and stored at high pressures. Different storage pressures have been developed in the industry ranging from 200 bar to 900-1000 bar for delivery at dispensers.

The storage tanks may be fixed such as bullets or portable such as baskets of bottles as shown in Fig. 1.

Fig.1: Example of a high-pressure storage tanks – bullets (left) and bottles (right).

2 Hydrogen safety

2.1 Hydrogen properties

Most of hydrogen hazards are directly linked to its properties. Therefore, the knowledge of the general physical and chemical properties, as well as flammability and ignition characteristics of hydrogen must be available to designers, operators, customers and first responders. Like gasoline or natural gas, hydrogen is a fuel that must be handled properly. It can be used as safely as other common fuels when simple guidelines are followed.

Hydrogen at ambient conditions [1], [2] are:

- The lightest molecule with a low viscosity and is therefore prone to leakage.
- 14 times lighter than air, so it rises at almost 20 meters per second and disperses rapidly. This buoyancy is a built-in safety advantage in an open environment but a potential concern in confined area.
- colorless, odorless, tasteless, and undetectable by human senses.
- non-toxic and non-poisonous; however, it can be an asphyxiant.
- widely flammable (between 4-75 % volume in air), so it should be safely stored and used in an area that is free of heat, flames, and sparks.
- non-corrosive, but it can embrittle some metals (i.e., cause significant deterioration of the metal's mechanical properties).

Under the optimal combustion condition (a 29% hydrogen-to-air volume ratio), the energy required to initiate hydrogen combustion is much lower than that required for other common fuels (e.g., a small spark will ignite it). But at low concentrations of hydrogen in air, the energy required to initiate combustion is similar to that for other fuels.

2.2 Safety objectives

The safety objectives in case of an accidental event are to ensure the protection of people in the vicinity while avoiding potential escalation to other units or to third parties.

There are safety challenges in the implementation of hydrogen production and storage solutions in urban and congested areas where there are many stakeholders. Hence risk analysis shall be carried out to identify credible accidental events and associated consequences in terms of fire and explosion.

2.3 Potential sequence of accidental events

Within the framework of the development of a temporary hydrogen pilot unit close to existing facilities, a hazard identification study was performed. Among the various hazardous release scenarios investigated, the consequences of the catastrophic rupture of a high-pressure hydrogen storage were judged critical for the third parties considering the current safety distances and corresponding impairment thresholds on vulnerable targets.

In particular, the hydrogen storage pressure burst will be potentially followed by a secondary explosion of the turbulent hydrogen-air mixture released following the mechanical one since ignition energy of hydrogen is very low and flammability limits are large. Consequently, two consecutive blast waves arising from the storage area will be generated and will hit the different critical targets identified during the risk analysis.

The re-evaluation of the effects of this scenario, considering the identified causes and the risk reduction measures already in place, did not allow the hazardous area to be reduced significantly. The qualitative assessment considered several other options such as a containment system surrounding the H_2 storage, but they were not retained due to major operational and maintenance constraints.

This paper focuses on the implementation of protective walls to reduce the overpressure levels from those accidental events on vulnerable targets.

A detailed quantitative analysis based on CFD simulations to compute the wave propagation from the pressure burst and the subsequent combustion of one or more H2 storage tanks, considering the benefits of the protective walls and other large buildings for different layout options and wall height was done. There was an iterative process to find the best position and height of the protective walls to limit the overpressure behind them to an acceptable level according to the expected resistance of the targets.

From the results of the FLACS CFD® simulations, a design solution made of Lego® like bricks was investigated using LS-DYNA®.

3 Explosion simulations with FLACS CFD®

3.1 FLACS CFD® software

FLACS (FLame ACceleration Software) CFD® software is a comprehensive software tool for modelling (dispersion and explosion) consequences in complex geometries for typical flammable and toxic release scenarios [3]. FLACS CFD® is developed and maintained by Gexcon since the 1980s (more than 40 years of development). This software is the industry standard for CFD gas explosion modelling and one of the best validated tools for modelling flammable and toxic releases in the technical safety context [4] [5] [6].
It is used extensively in the Oil and Gas and Process industries (especially for offshore facilities) and also increasingly in the nuclear industry, in facilities with dust explosion potential and many other fields.

FLACS CFD® solves for the velocity components on a staggered grid, and for scalar variables, such as density, pressure and temperature, on a cell-centered grid. The accuracy of the FLACS CFD® solver is second order in space and first/second order in time.

Fig.2: Example of a hydrogen explosion large scale experiments on Gexcon test site

The main characteristics of the solver are:

- Transient or steady-state simulations
- Compressive or un-compressive flows
- Time-stepping according to CFL condition (Courant Friedrichs Lewy Condition) both for wave propagation and flows
- U-RANS resolution: Reynolds Average Navier-Stokes (reactive) or EULER (non-viscous adiabatic flows)
- k-epsilon CFD model, which assumes isotropic turbulence
- Corrected Flow Transport (CFT) algorithm for far field wave propagation
- Porosity Distributed Resistance (PDR) Concept

With this PDR approach, large objects and walls are represented on-grid (explicit resolution of large eddies), whereas smaller objects are represented sub-grid. The preprocessor Porcalc reads the grid and geometry files and assigns volume and area porosities to each rectangular grid cell. In the simulations, the porosity field represents the local congestion and confinement, and this allows sub-grid objects to contribute with flow resistance (drag), turbulence generation and flame folding in the simulations. Empirical correlations from experiments are implemented for efficient modeling of the flame structure. This is a key strength which allows to use FLACS CFD® at an industrial scale, while keeping accurate results in a reasonable time scale if grid rules restrictions described in Manual are kept.

When it comes to describing real industrial systems, it is important for users of advanced CFD tools to keep in mind that most simulations are inherently 'under-resolved', and that a significant degree of sub-grid modelling is required. This implies that solutions may not converge as the spatial or temporal resolution increases, and it is important to follow the guidelines provided by the software vendor.

FLACS CFD® does not model the transition from deflagration to detonation, however, to estimate the probability of this phenomenon and to determine whether it takes place, the spatial pressure gradient could be observed. Indeed, just before this transition, the pressure increases dramatically without geometrical reason. Therefore, a strong gradient may be an early indicator of potential detonation transition. The DPDX parameter in FLACS CFD®, describes the normalized spatial pressure gradient across the flame front.

3.2 3D Model preparation

According to the objectives of the study, the 3D modelling effort was limited and spent on large buildings structures that will affect the diffraction of the blast wave from the storage area. Critical targets and protective walls were implemented while pipework, small equipment and frame structures were not represented in the model. Due to the resolution scheme and to avoid convergence issues, the geometry is slightly modified to fit properly in the cartesian mesh. Hence tilt walls are modelled as staircases. The model is show in Fig 3.

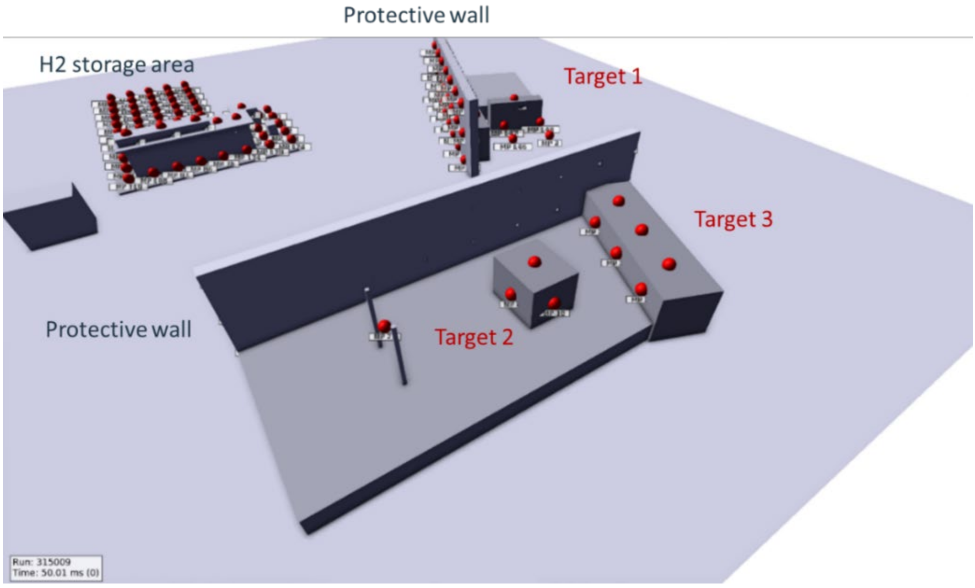

Fig.3: 3D geometry model setup in FLACS CFD® and monitor points (in red)

Monitor points (red points) are spread onto the hydrogen storage area, protective walls and also on the critical targets.

3.3 Pressure burst simulations

For sake of simplicity and according to software limitations, the pressure burst is modelled as high-pressure hydrogen bubble corresponding to the storage volume and operating pressure. The initial high-pressure region follows the cartesian grid of FLACS CFD® with a minimum number of cells for proper solving. The computational domain is limited to the near field of the storage area, encompassing the adjacent buildings, which might have some impact on the diffraction of the blast wave.

A mesh sensibility study was done to ensure that the peak overpressure and impulse were correctly captured as shown in Fig. 4 and Fig. 5. Finally, the grid cell is cubic with a 10 cm size. The pressure, impulse and dynamic pressure are recorded but also concentration, volume fraction, turbulence of hydrogen is also captured for the subsequent combustion phase.

The time step is automatically calculated using the Courant Friedrichs Lewy criterion both for flows and wave propagation in fluids.

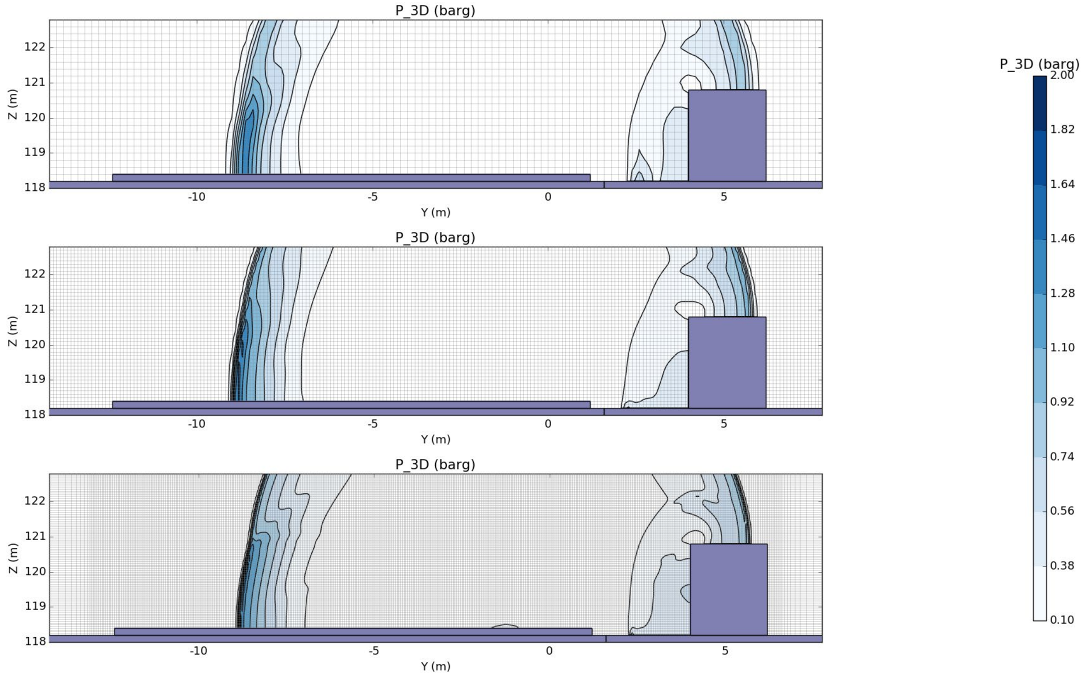

Fig.4: 2D Contours of overpressure for different cell sizes (20 cm,10 cm, 5 cm)

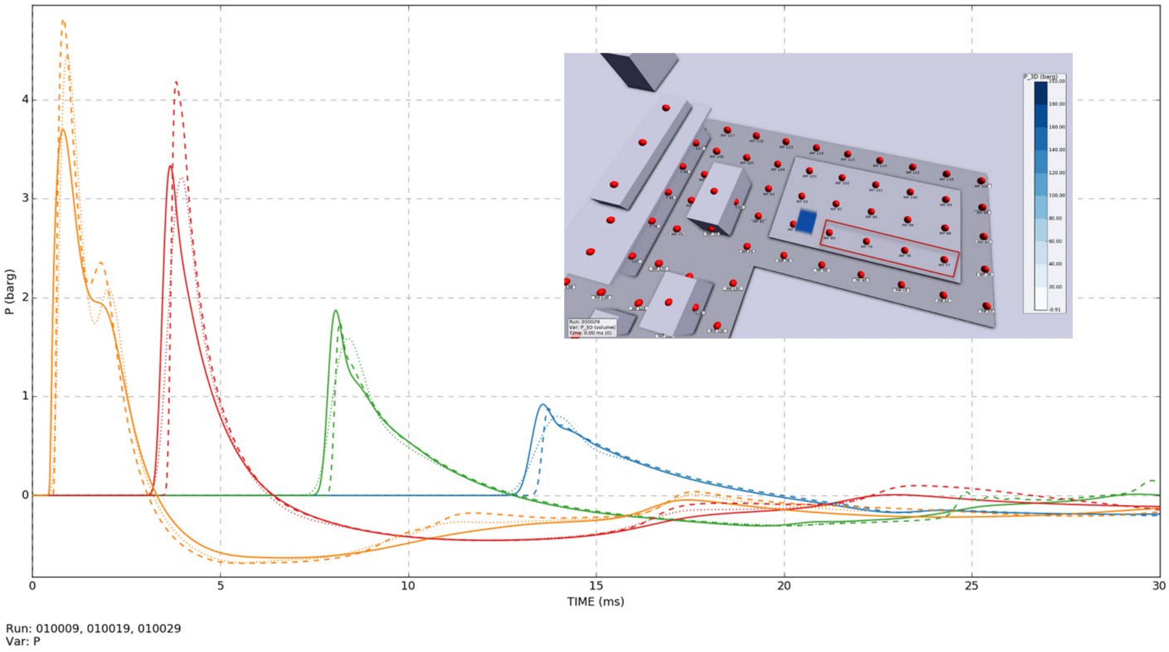

Fig.5: Time historiy at selected monitor points for different cell sizes FLACS CFD®

When the blast wave reaches the limits of the storage area, the simulations are dumped for the next step of the simulation process and are remapped on a wider computational domain, with a larger grid size in accordance with the combustion solver requirements.

3.4 Gas explosion CFD simulations

While premixed combustion under constant volume or constant pressure conditions is straightforward to describe, gas explosions in industrial environments are complex phenomena. The key physical phenomenon to model is the positive feedback loop between expansion-generated flow and increased rate of turbulent combustion, which leads to flame acceleration, pressure build-up and generation of blast waves. The hydrogen-air deflagration simulations are performed with FLACS CFD® with the compressible combustion solver described earlier.

Multiple ignition points and timings are considered to maximize the flame travel path and subsequent acceleration through the flammable gas cloud which generates the secondary blast wave. Fig. 6 is showing the generation of two blast waves from the storage area: the first wave from the pressure burst and the second one resulting from the gas explosion.

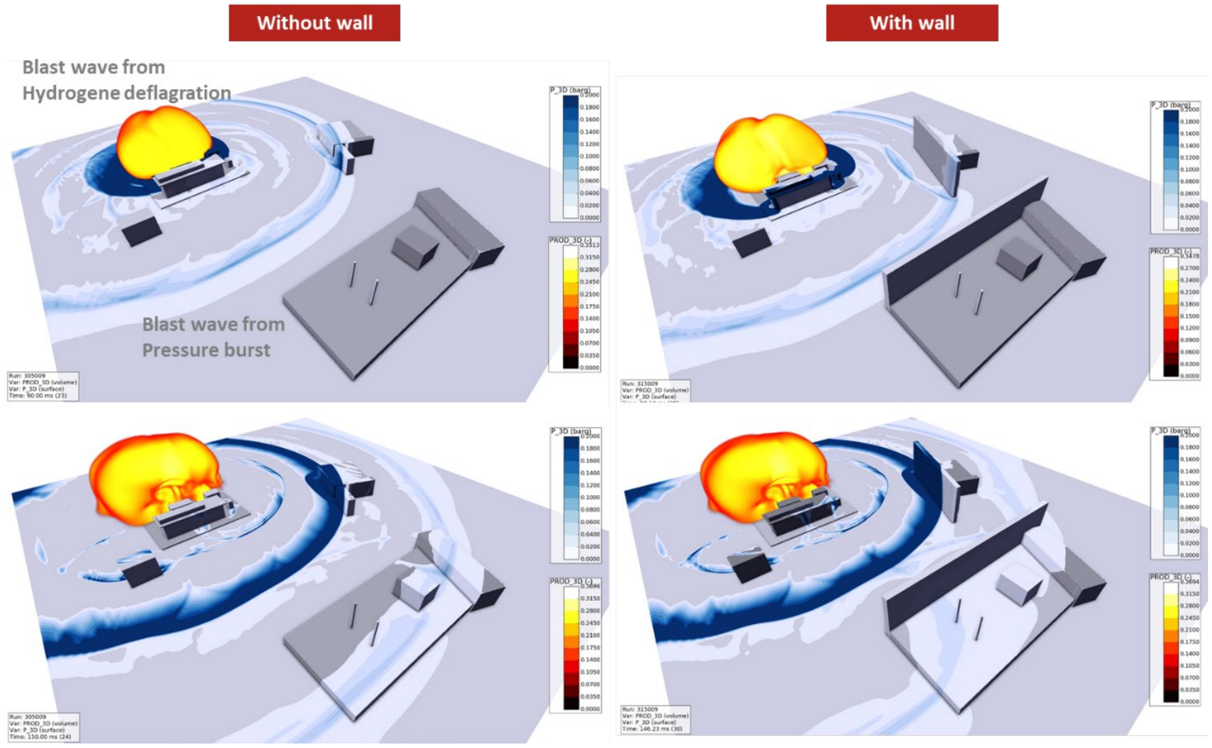

Fig.6: Contours plots of the two blast waves from pressure burst and gas explosion without or with a wall at different time steps – overpressure on surfaces (in blue) and iso contours of combustion products (in red to yellow).

Time history profiles at selected location behind the protective walls are shown in Fig. 7. It is confirmed that the pressure burst phenomena in this case is weaker than the subsequent gas explosion phenomena. Hence these two phenomena shall be considered together in the safety analysis.

The attenuation of the blast wave behind the protective walls is also highlighted compared to the base case without any protection of the targets. For the configuration studied, the FLACS CFD® simulations have shown that a 40% reduction was expected for the 6 m high wall and 60% for the 8 m high wall. Maximum contours of overpressure over time are shown in Fig. 8.

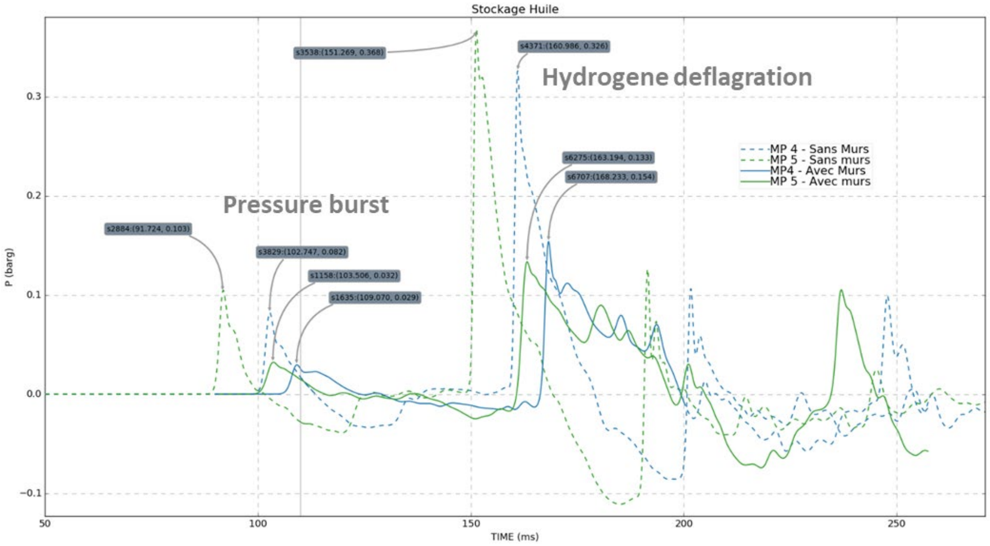

Fig.7: Time historiy on selected points behind protective walls

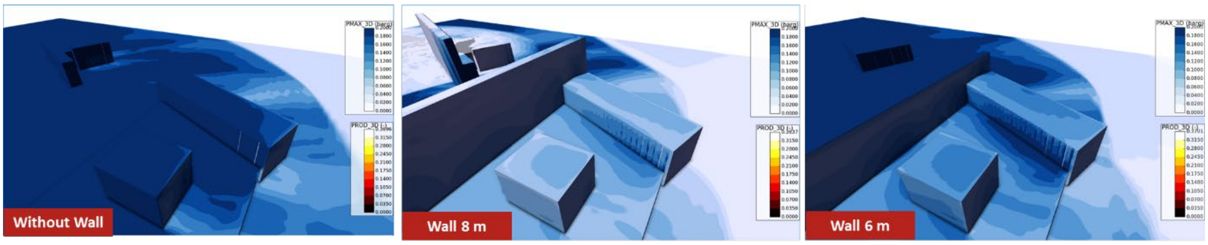

Fig.8: Comparison of base case (left) and protective walls simulations (middle and right)

3.5 Explosion load mapping from FLACS CFD® to LSDYNA

In an advanced risk analysis approach, numerical solutions for both the fluid domain (explosion calculations) and the structural domain (blast response calculations) are based on a three-dimensional model of the relevant geometry.

For applications dealing with reinforced concrete structures, a so-called "one-way-fluid-structure-interaction" approach can be adopted: the displacements characterizing the structural response are small with respect to the typical dimensions in the geometry, meaning that the modifications of the boundaries in the fluid domain are negligible; the fluid flow is therefore not influenced by the structural response. This implies that it is possible to decouple the fluid-structure-interaction problem, by first solving the fluid dynamic equations in the fluid domain, obtaining the fluid dynamic solution on the boundary (in terms of pressure distribution), and then solving the structural response equations adopting the fluid boundary pressures as external loads acting on the structural domain.

The general approach in the industry is to get time history from the CFD simulations and simplify the transient Design Accidental Loads (DAL) to triangular loads before applying them in the Finite Element analysis. Typical concepts commonly (and compulsorily) assumed in other approaches (such as dynamic load factor for quasi-static approach, or equivalent pulse determination, or reflection coefficient when using blast decay schemes for far field explosion pressure estimation), do not apply here.

Simplified downscaled expression of DAL may be non-conservative, inefficient or difficult to justify while the benefits of CFD tool is lost. In the approach here, the pressure time-and-space distribution is integrally calculated in the computational fluid dynamic (CFD) task and mapped onto the finite element (FE) computational model for structural response analysis.

The described approach does not require any assumption, simplification, or manipulation for the blast load to be assumed.

From the monitored points spread onto the protective walls (Fig. 9), the effective (reflected) overpressure time history loads (Fig. 10) are computed and used as an input to LS-DYNA® simulations.

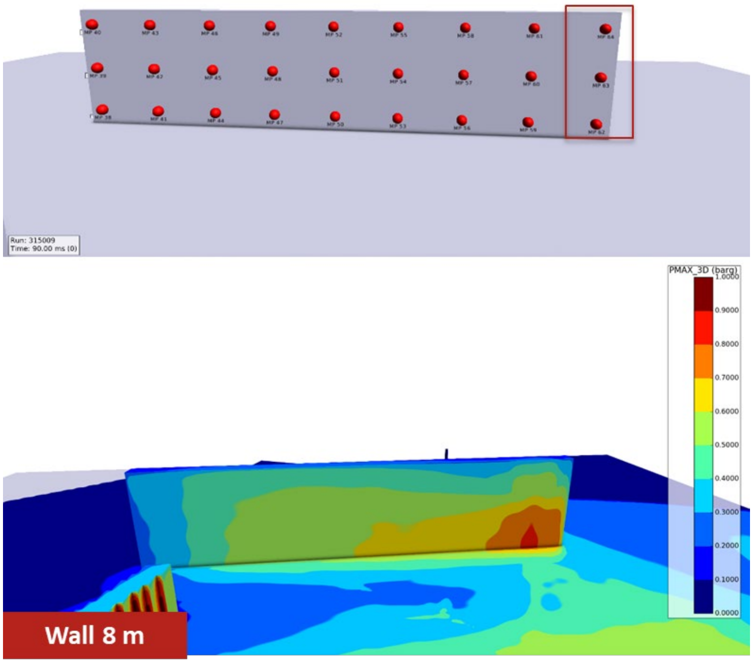

Fig.9: Monitored points on protective walls (top) and contours of maximum effective pressure loads for the response analysis

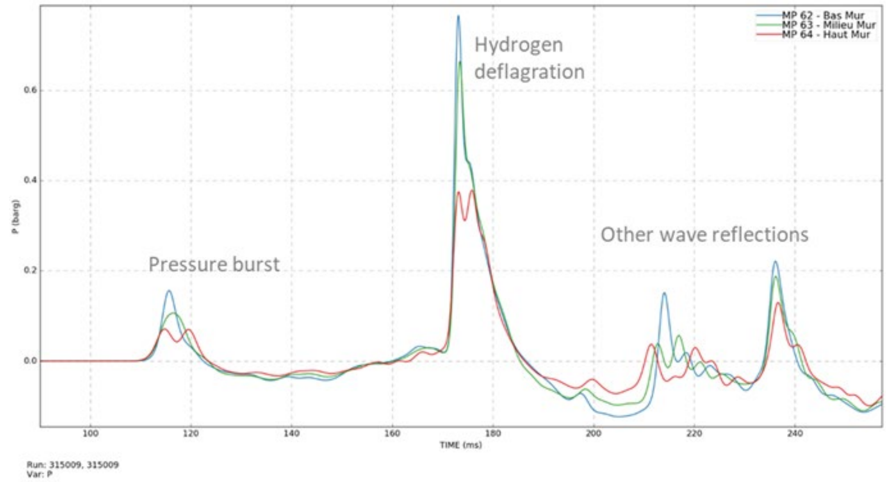

Fig.10: Time history of explosion loads for the 3 selected monitored points on the wall (bottom, middle and top)

4 Response of the protective walls with LS-DYNA®

The objective of the simulation is to predict the overall stability of the concrete wall after the explosion event. The following section describes the general modeling of the numerical LS-DYNA® model.

Since it is a temporary facility, a flexible and removable protective solution was chosen.

4.1 Model Geometry and discretization

The wall consists of concrete blocks stacked on top of each other. The blocks fit together through studs like the well-known LEGO® bricks as shown in Fig. 11. In this way no mortar is necessary.

Fig.11: Example of a concrete block (left) and assembly (right)

Considering the cantilever protective wall and the maximum overpressure gradient expected, only a representative strip of the wall is modelled in LS-DYNA®.

The height of the modelled wall is 8 m which results in the stacking of 10 bricks. The width of the modelled wall is 2.3 m and includes 1.5 bricks in each layer. One layer of brick through the thickness is modelled as shown in Figure 15. The nominal brick dimensions are specified as 1.6x0.8x0.8 m^3.

Each brick is initially meshed with an element length of 0.04 m for the studs and around 0.1 m elsewhere. The meshing contains only hexahedral elements, and their formulation is the fully integrated S/R solid (**`ELFORM=-2`** in **`*SECTION_SOLID`**). A finer mesh has been tested and yields similar force and displacement results. Both meshes are shown in Fig. 13.

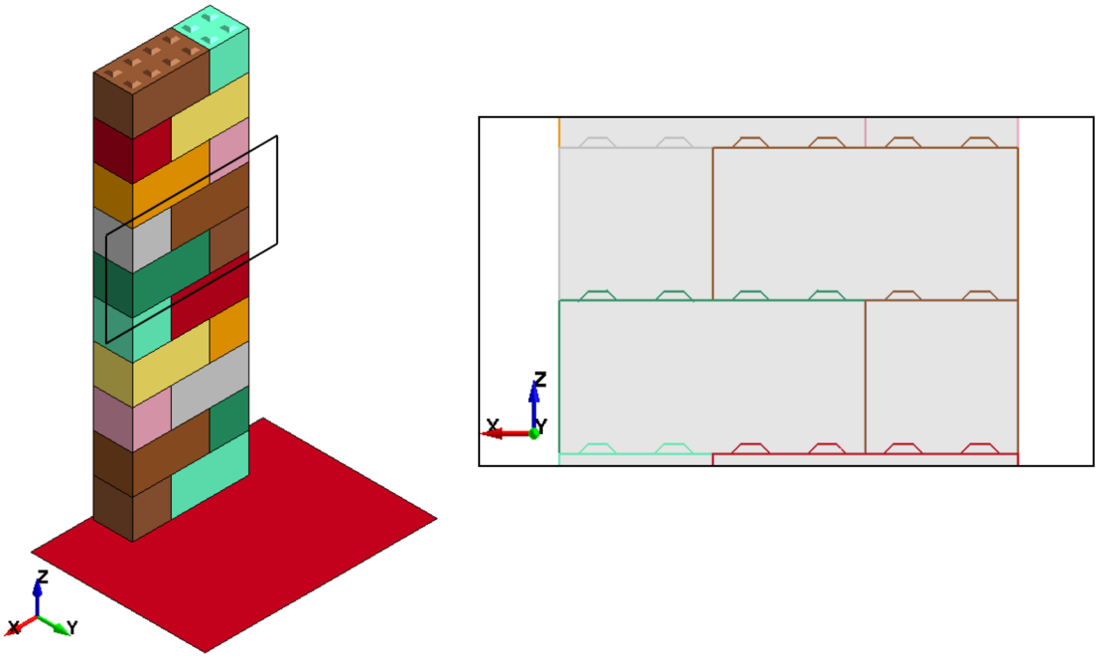

Fig.12: Model brick wall (left) and close up view of the wall stacking (right)

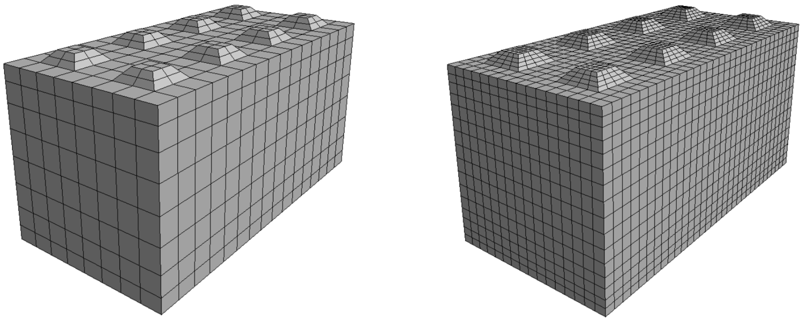

Fig.13: Reference brick mesh with 2048 elements, 0.04 m for the studs, ~0.1 m elsewhere (left) and finer brick mesh with 16384 elements, 0.02 m for the studs, ~0.05 m elsewhere (right)

4.2 Material modeling

4.2.1 Bricks

Because little information is known about the properties of the concrete, it has been decided to use the “simple input concrete models” available in LS-DYNA®, with automatic material parameter generation based on unconfined compressive strength:

- **`*MAT_PSEUDO_TENSOR`** (**`*MAT_016`**),
- **`*MAT_CONCRETE_DAMAGE_REL3`** (**`*MAT_72R3`**) (Karagozian and Case Concrete model),
- **`*MAT_CSCM_CONCRETE`** (**`*MAT_159`**) (Continuous Cap Surface Concrete model).

The reasons to keep these 3 constitutive models are explained in an article by Schwer [7]

- The shear failure surfaces of these concrete models are quite different even if the same unconfined compressive strength is defined.
- A comparison of the results will indicate if the stability of the model is sensitive to the material model.

For a deeper study of these material laws, the interested reader is referred to the current LS-DYNA® Keyword’s manual [8].

4.2.2 Ground

The ground is modelled as rigid **`*MAT_RIGID`**.

4.3 Wall assembly and contact modelling

Since different sizes of wall may need to be tested quickly, a user-defined python script is executed to create the wall in a LS-DYNA® solver deck. The user just needs to fill in the overall dimensions of the wall and the location of the two nominal bricks LS-DYNA® inputs. This script takes this data and translates it to LS-DYNA® **`*INCLUDE_TRANSFORM`** and **`*DEFINE_TRANSFORMATION`** keywords. In this manner, each basic brick is imported repeatedly.

In addition, the script retrieves and defines all the different sets of entities which are needed to define the boundaries and the contact. For the latter, only one single surface contact is needed to take care of the full wall. **`*CONTACT_AUTOMATIC_SINGLE_SURFACE`** is used for this purpose and **`*CONTACT_FORCE_TRANSDUCER_PENALTY`** are defined to measure the contact force for each layer. The friction coefficient is set to 0.4.

4.4 Boundaries conditions

The simulation is divided into three steps: Gravity, stabilization, and explosion loading. The following section describes each step. The explicit method is used for the three steps and no mass scaling is defined.

4.4.1 Gravity

The gravity is specified as a sinusoidal function of time, is set to zero at the beginning, reaches 9.81 m/s^2 after 0.25 s and is maintained for the remainder of the simulation. Moreover, some mass-weighted damping is defined through the keyword **`*DAMPING_PART_MASS`** to remove the oscillations in displacements and force time histories. To define the damping coefficient D, a first simulation without any damping has been launched to determine the lowest frequency mode of interest [9].

$$D = 2\omega_{min} \tag{1}$$

where ω_{min} is that lowest frequency in units of radians per unit time.

4.4.2 Stabilization

The mass damping is also specified as a sinusoidal function of time and is set to zero after achieving a steady state condition. In this manner, it will not inhibit physical motion afterwards. This is the goal of the stabilization step. The Figure 17 shows that at the end of the stabilization, the system has reached a steady state condition.

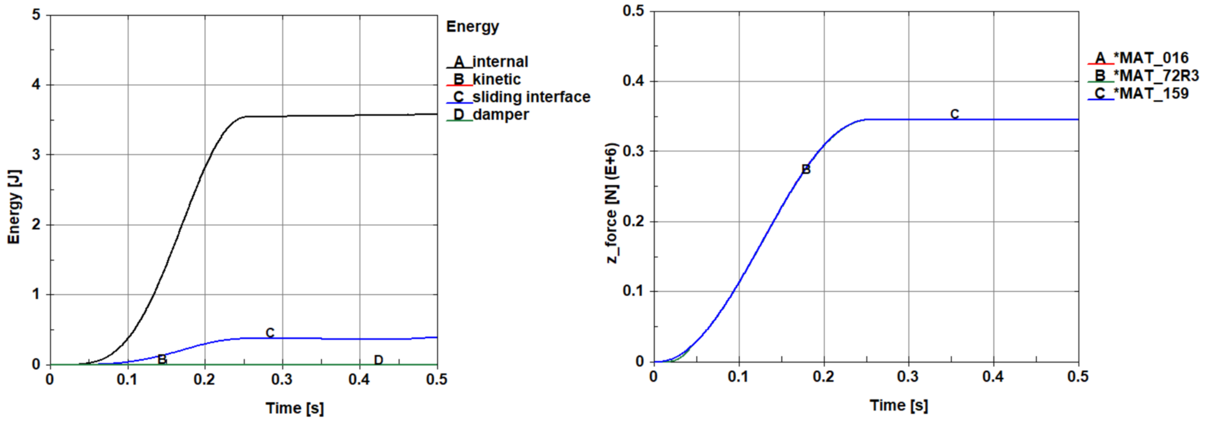

*Fig.14: Energy balance for **`*MAT_159`** (left) and reaction force between the wall and the ground for each model (right) from the beginning to the end of the stabilization*

4.4.3 Explosion

The Y faces (see Fig. 18) are transiently loaded according to the profiles obtained from FLACS CFD® using the **`*LOAD_SEGMENT`** keyword.

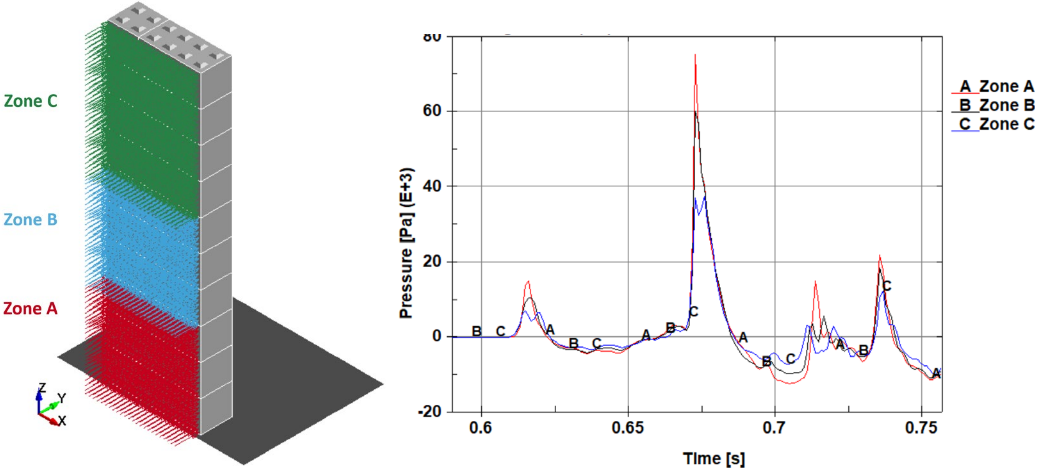

Fig.15: Definition of the zones A, B and C (left) and the corresponding load pressure profiles in function of time obtained from FLACS CFD® for each zone (right)

To assess the stability of the wall, the Y-displacement of the highest node on the wall is analyzed (see Figure 19). The maximum displacement for all material model is 14 mm. Then, the wall oscillates but does not fall and the displacement amplitude is reduced gradually. In this model, the energy dissipation is only due to the friction. In addition, neither did a slight stiffness-proportional damping via **`*DAMPING_PART_STIFNESS`** nor a viscous damping coefficient (tested with **`VDC=0, 20`** or **`40%`**) in the contact have a significant influence on these oscillations.
If the impulsive loading was more severe, more differences should be noticed between the different concrete model.

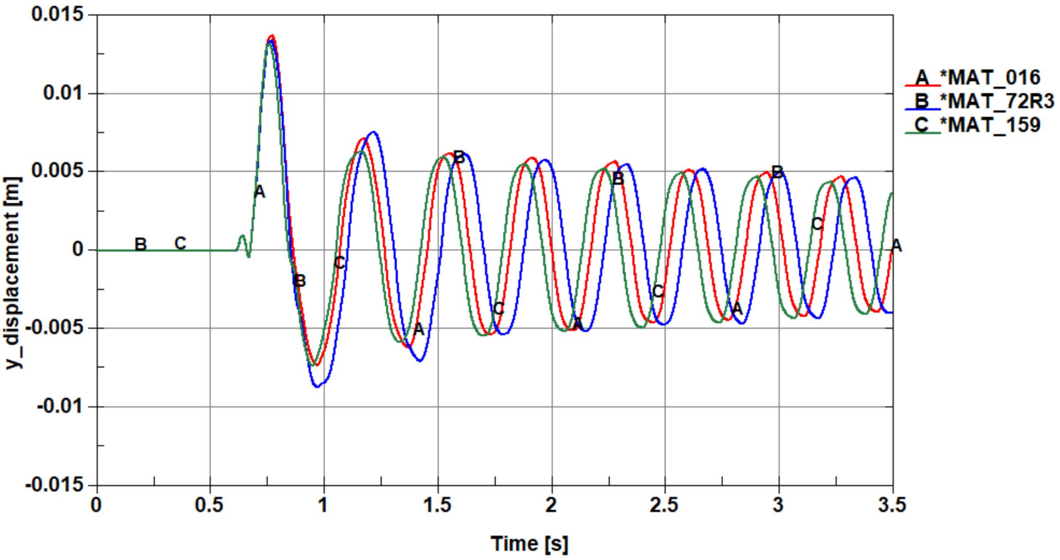

Fig.16: Y-displacement on top of the wall in function of time for the 3 models

The LS-DYNA® simulations performed on a representative strip of the cantilever brick wall demonstrated that the 8 m height wall can withstand the actual overpressure loads from the catastrophic rupture of the hydrogen storage with limited oscillations. Stability is also ensured for the 6 m high wall.

5 Conclusions and further work

The consequences of a catastrophic rupture of a hydrogen storage were assessed in terms of overpressure for both the initial pressure burst and the subsequent turbulent hydrogen deflagration. The simulation work performed with FLACS CFD® enabled the quantification of the shadowing effects of the protective walls on the critical targets and hence “optimal” dimensions and location considering the site constraints. The results of the CFD simulations have provided credible time history overpressure loads as an input for the response work with LS-DYNA®. A brick model generation was successfully developed in LS-DYNA® thanks to Python® scripting. This proof of concept enables a wide range of applications for temporary protective structures.

Finally, the present work has shown the benefits of combining FLACS CFD® and LS-DYNA® for hydrogen safety applications.

6 Summary

In the objective to mitigate the effects of climate change, hydrogen is pushed forward in many countries as a new energy carrier. Even if hydrogen is well-known and used in the industry, it shall be handled with care due to its high flammability properties. Hence the development of hydrogen production and high-pressure storage facilities in existing congested and built environment with many stakeholders requires the performance of hazards studies to define adequate risk reduction measures.

In this article the design of a temporary protective wall against the overpressure effects from the catastrophic rupture of high-pressure hydrogen storage and subsequent hydrogen-air deflagration was evaluated. The CFD simulations were performed with FLACS CFD® while the response simulations were performed with LS-DYNA® on a representative stacked brick assembly.

The LS-DYNA® brick model was developed using Python scripts which enable the assessment of various brick arrangements in a flexible and efficient way. The methodology was applied on simple cantilever walls in this “proof of concept” study, but it could be enhanced for more complex situations in which such protective walls might be necessary for safety purposes, including impact of projectiles.

According to the results of the simulations, the response of the wall was satisfactory for such magnitude of overpressure with small self-damping oscillations thanks to friction between blocks. The implementation of such a design solution would be efficient since it does not require too much preparation and construction means on site.

The results have also shown the benefits of combining FLACS CFD® and LS-DYNA® together to evaluate the whole sequence of the accidental event combining a primary blast wave from the pressure burst and a secondary blast wave from the hydrogen deflagration.

7 Literature

[1] V. Molkov, Fundamentals of Hydrogen Safety Engineering, Bookboon, 2015.

[2] NFPA, «NPFA 2 - Hydrogen Technologies Code,» NFPA, 2020.

[3] Gexcon AS, «FLACS CFD v21.1 User's manual,» Gexcon AS, 2021.

[4] P. Middha, «Development, use and validation of the CFD tool FLACS for Hydrogen safety studies,» 2010.

[5] Gexcon, «Experimental investigation of vented hydrogen deflagrations in containers - Phase 1 : Homogeneous mixtures,» HYSEA - Fuel Cells and Hydrogen 2 Joint Undertaking, 2016.

[6] GEXCON, «FLACS Validation cases for Hydrogen explosions,» Janv. 2020.

[7] L. Schwer, «Simple Input Concrete constitutive models : an ilustration of Brick Wall & Concrte Cylinder Perforation,» chez *10th International LS-DYNA Users Conference*, 2008.

[8] ANSYS LST, LS-DYNA Keyword User's Manual - Volume II, 2021.

[9] ANSYS LST, LS-DYNA Keyword user's manual - Volume I, 2021.