STRUCTURAL RESPONSE FOR VENTED HYDROGEN DEFLAGRATIONS: COUPLING CFD AND FE TOOLS

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ABSTRACT

This paper describes a methodology for simulating the structural response of vented enclosures during hydrogen deflagrations. The approach adopted entails full spatial mapping of explosion loads predicted with the computational fluid dynamics (CFD) tool FLACS-Hydrogen to the non-linear finite element (FE) IMPETUS Afea solver. The modelling involves one-way coupling of pressure loads taken from either experiments or CFD simulations to the FE solver. The performance of the combined model system is evaluated for vented hydrogen deflagrations in 20-foot ISO containers. The work is part of work package 3 (WP3) in the project 'Improving hydrogen safety for energy applications through pre-normative research on vented deflagrations' (HySEA).

1. INTRODUCTION

It is common practice in industry to install refuelling stations, fuel cell backup systems, electrolysers and other equipment for hydrogen energy applications in containers or smaller enclosures. Explosions and fires represent an inherent hazard in such systems, and explosion venting is often used to reduce the risk of accidental hydrogen deflagrations in confined systems to a tolerable level. The main objective of the project *Improving Hydrogen Safety for Energy Applications through pre-normative research on vented deflagrations*, or HySEA (www.hysea.eu), is to facilitate improvements to international standards for the design of explosion venting devices. The members of the HySEA consortium are Gexcon (coordinator), University of Warwick (UWAR), University of Pisa (UNIPI), Fike Europe, Impetus Afea and Hefei University of Technology (HFUT). This paper presents a methodology for one-to-one coupling of explosion loads, taken from either experiments or computational fluid dynamics (CFD) simulations, to a finite element (FE) model. This would allow researchers and engineers to estimate the structural response of enclosures during vented hydrogen deflagrations, and hence to design venting devices suitable for industrial applications. The coupling methodology used in this study was first proposed and demonstrated for an offshore process module by Salaün *et al.* [1].

2. EXPERIMENTS

The experimental setup consisted of a standard 20-foot ISO container, fitted with a steel frame for instrumentation and obstacle support, and venting either through the container doors or through vent openings in the roof [2-3]. Figure 1 shows a container with a displacement sensor (on the yellow pole).

Figure 1: ISO container with displacement sensor and target plate.

Figure 2 shows vertical cross-sections of containers, illustrating available vent openings (door or roof), obstacle positions (1-3), and ignition positions (A and B) on the left, and an example experimental configuration with a pipe rack (P) in position 1 (P1) and a bottle basket obstacle (B) in position 3 (B3).

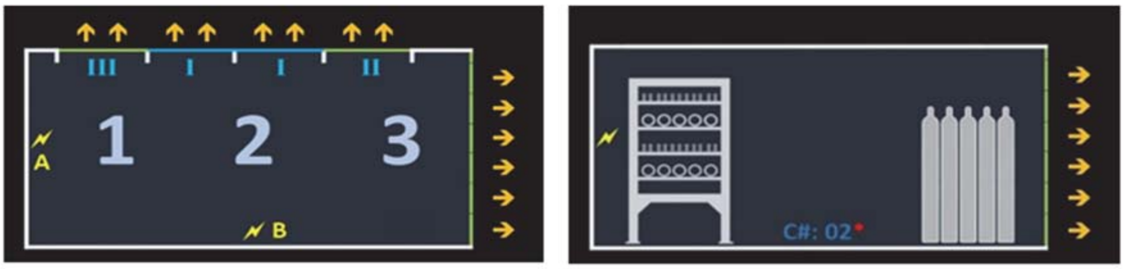


Figure 2: Nomenclature (left) and example configuration the ‘P1B3’ for test 14 (right).

Figure 3 illustrates the positions of the internal pressure sensors (P1-P8), the external pressure sensors (P9-P11), and the displacement sensors (D1-D2). Two Acuity AR700-50 Laser displacement sensors, normally operated at 10 kHz, measured the dynamic response of the side walls of the containers [2-3].

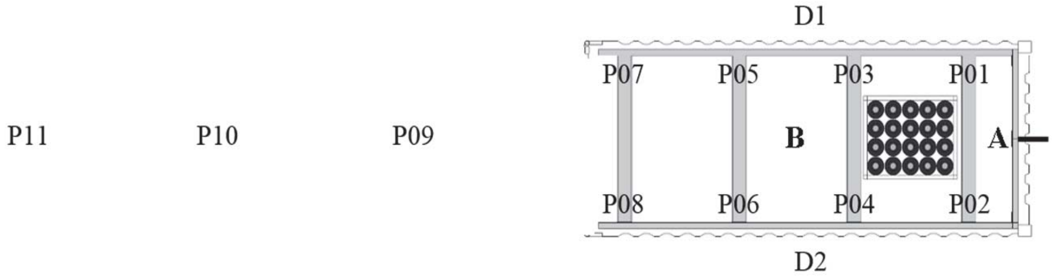


Figure 3: Positions for pressure and deflection sensors.

Tables 1 and 2 summarize the experimental conditions for tests with venting through the doors and roof, respectively [2-3]. The test numbers highlighted with bold font indicate experiments selected for test cases in the present study. The symbol * indicates tests where the container was severely damages, and replaced. Phase 1 of the experimental campaign in 20-foot ISO containers consumed five containers. Tests 1-6 were part of the first HySEA blind-prediction study.

Table 1: Summary of the experiments with venting through the container doors [2-3].

Configuration	Test	A_v (m^2)	[H$_2$] (vol.%)	Ign. pos.	$P_{\text{red, max}}$ (bar)
Frame only (FO), doors open (O)	**01**	5.64	15	A	0.040
	02				0.047
	05				0.039
Bottle basket (B1), doors open (O)	**03**	5.64	15	A	0.077
	04				0.064
	06				0.045
	10	5.64	18	A	0.130
	07	5.64	21	A	0.190
	08	5.64	24	A	0.390
Bottle basket (B1), doors closed (C)	09*	0.00	24	A	1.447
Pipe rack (P1), doors open (O)	11	5.64	15	A	0.050
	12	5.64	18	A	0.120
	13	5.64	21	A	0.279
Pipe rack and bottle basket (P1 B3), doors open (O)	14*	5.64	21	A	0.939

Table 2: Summary of experiments with venting through the container roof [2-3].

Configuration	Test	A_v (m^2)	[H_2] (vol.%)	Ign. pos.	$P_{red,\ max}$ (bar)
Frame only (FO), perforated plastic film (O)	25	4.0	21	B	0.146
	21	6.0	21	B	0.120
	16	8.0	21	B	0.190
Pipe rack (P2), perforated plastic film (O)	24	4.0	21	B	0.150
	22	6.0	21	B	0.142
	17	8.0	21	B	0.124
Pipe rack (P2), perforated plastic film (O)	34*	8.0	42	B	1.076
Pipe rack (P2), perforated plastic film (O)	**29**	4.0	24	B	0.414
	23	6.0	24	B	0.168
	19	8.0	24	B	0.136
Frame only (FO), commercial vent panels (P)	32	4.0	21	B	0.214
	26	6.0	21	B	0.245
	15	8.0	21	B	0.191
Pipe rack (P2), commercial vent panels (P)	33	4.0	21	B	0.261
	27	6.0	21	B	0.301
	31				0.249
	18	8.0	21	B	0.234
	30				0.214
Pipe rack (P2), commercial vent panels (P)	28*	6.0	24	B	0.45 / 0.73 ?
	20*	8.0	24	B	0.334

3. SIMULATIONS

This section describes the CFD tool FLACS-Hydrogen and the IMPETUS Afea FE solver.

3.1 FLACS-Hydrogen

FLACS™ (FLame ACceleration Simulator) is a finite volume CFD tool that is widely used to simulate the consequences of industrial accident scenarios that involve release and dispersion of hazardous material, fires and explosions [4]. The numerical solver Flacs-2 for the software tool FLACS is based on a structures Cartesian mesh, and belongs to the porosity/distributed resistance (PDR) family of CFD solvers [5-6]. FLACS uses two-equation Reynolds-averaged Navier Stokes (RANS) turbulence models coupled with a premixed combustion model to simulate turbulent reacting flows. Empirical approximation of selected model components allows for a significant increase in computational speed. FLACS-Hydrogen is essentially a subset of FLACS for hydrogen applications [7-9].

3.2 Simulation setup

Figure 4 illustrates the geometry model for one of the container experiments in FLACS (‘B1’ scenario).

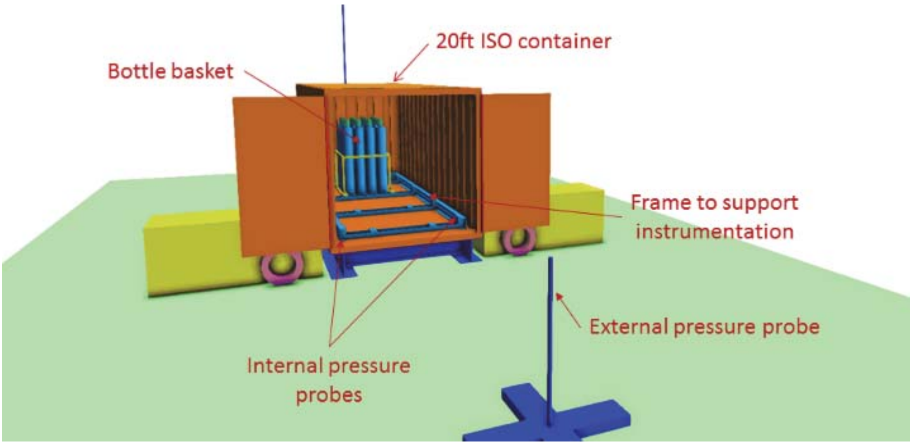


Figure 4: Geometry model with bottle basket in inner position (B1).

For the simulations of vented deflagrations in 20-foot ISO containers, Gexcon used a computational domain with dimensions 30 m × 12.5 m × 9 m, mesh sizes 0.1 m and 0.05 m, and PLANE_WAVE boundary conditions. The explosion loads on the walls and roof were captures with pressure panels.

3.3 IMPETUS AFEA FE solver

The IMPETUS Afea Solver is a commercially available system for non-linear explicit finite element analysis (NLFEA). The solver is primarily developed to predict large deformations of components exposed to extreme loads. It offers unique higher-order solid element technology, explicit time integration and GPU adaptation for enhanced computational speed. The formulation is purely Lagrangian. The finite element and contact calculations are carried out in double precision. The higher order elements lead to high accuracy even for highly distorted meshes. The materials are modelled according to minimum requirements with regards to strength and ductility [10-11]. A ductile damage model is used to account for stress tri-axiality and plasticity and assess the failure of the material.

3.4 CFD/FE model

Figure 5 illustrates the mapping of experimental data to the geometry model used by the IMPETUS Afea solver. The model consists of quadratic hexa-elements, applies a symmetry plane to limit computational costs, and the lower corners are clamped. The container doors were not included in the FE model, since they were open during the experiments. The steel parts of the container were modelled as 335 steel, using a model from IMPETUS material library. The FE models applies the full spatial mapping of transient overpressures from FLACS simulations, captured by pressure panels. The methodology entails a one-to-one CFD-NLFEA job solution scheme [1].

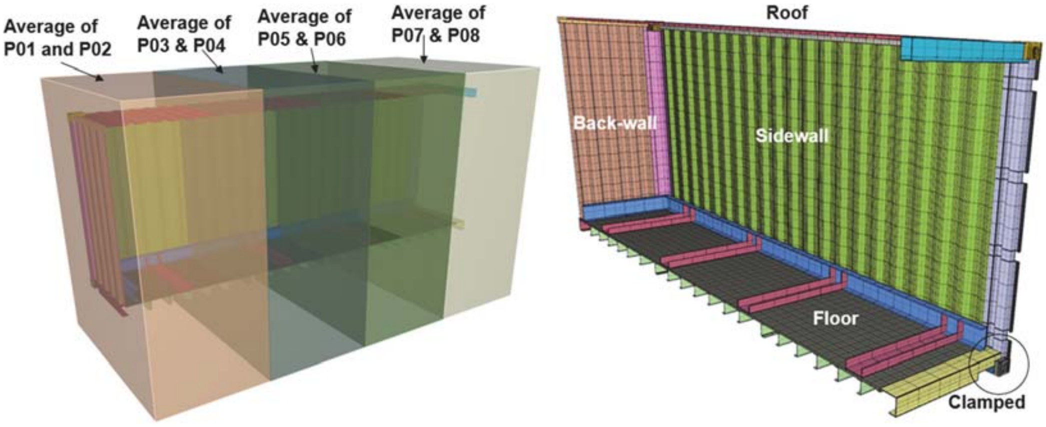


Figure 5: Mapping of experimental pressure data to FE model.

4. RESULTS AND DISCUSSION

4.1 Results from blind-prediction study

Impetus performed FE analysis for an empty enclosure (tests 01, 02 and 05) and an enclosure with a bottle basket obstacle (tests 03, 04 and 06) as part of the first HySEA blind-predictions exercise (see Table 1). Figure 6 shows the pressure-time histories simulated with FLACS-Hydrogen for an empty container (frame only) at pressure panels placed at four locations: side-wall, back-wall, roof and floor, and Figure 7 shows the structural response predicted by the FE solver. The maximum displacement predicted by the FE solver is 17 mm, which is comparable to the experimental results for the three repeated experiments (tests 1, 2 and 5): 20, 20 and 42 mm. Figure 8 shows the contours of the simulated displacement on the side-wall. The maximum displacement occurs near the centre of the wall.

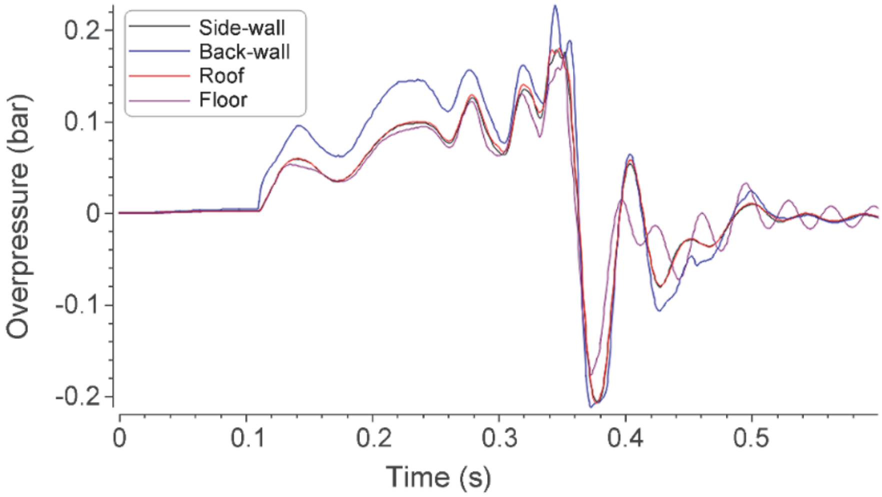


Figure 6: Pressure-time data from FLACS-Hydrogen for tests 1, 2 and 5.

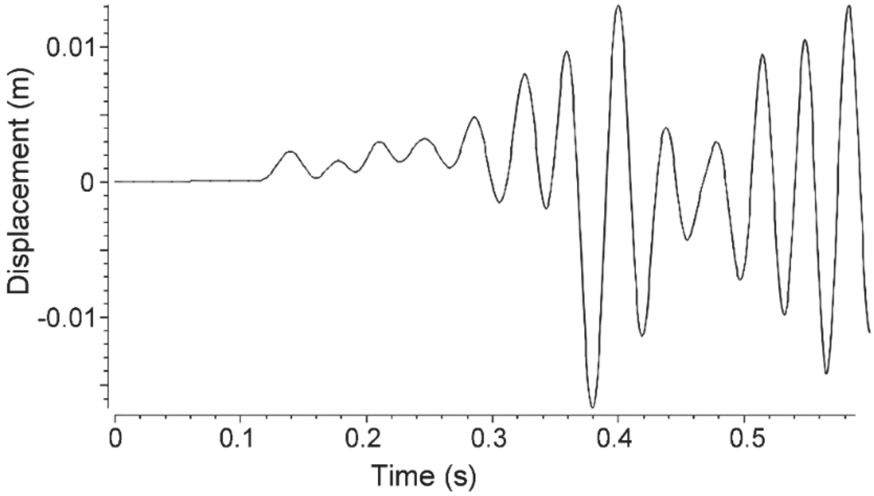


Figure 7: Displacement-time data from FE solver on central side-wall for tests 1, 2 and 5.

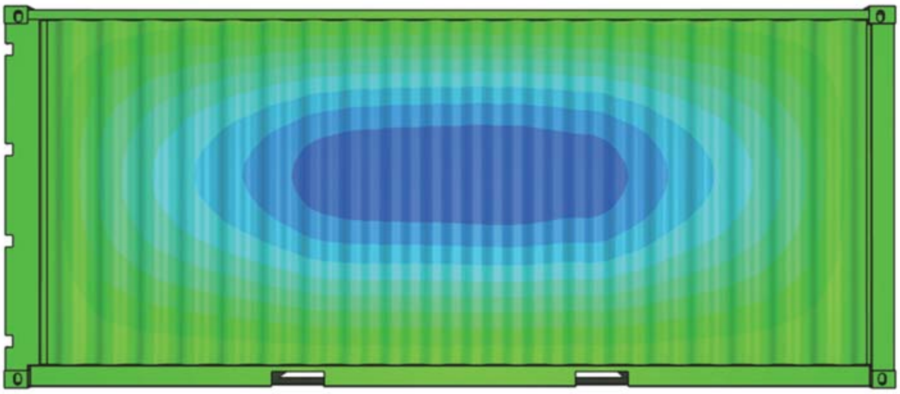


Figure 8: Displacement data contours on the side-wall for tests 1, 2 and 5.

Figure 9 shows pressure-time histories simulated with FLACS for a container with a bottle basket in position 1 (i.e. configuration B1), and Figure 10 shows the corresponding displacement computed by the IMPETUS Afea FE solver. The congestion results in a more violent explosion, and the FE model predict a maximum displacement of 73 mm. The corresponding deflections measured in the experiments were 105, 75 and 36 mm (test 3, 4 and 6). It is likely that the significant spread in the experimental results is caused by permanent deformation of the steel structure, since the same container was used in all tests (Table 1).

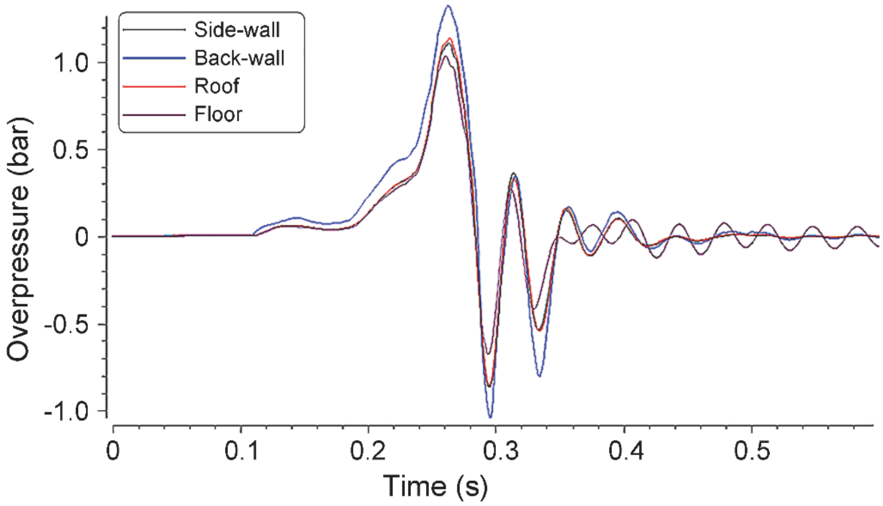


Figure 9: Pressure-time data from FLACS-Hydrogen for test 3, 4 and 6.

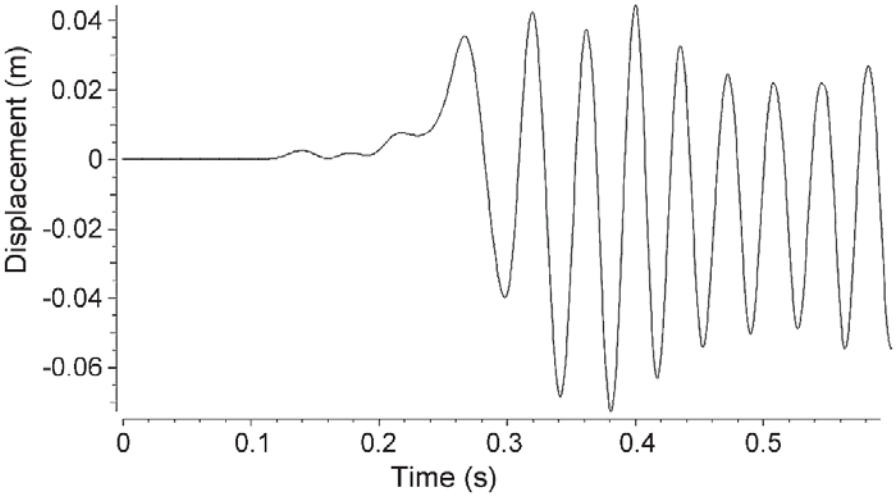


Figure 10: Displacement-time data from FE solver on central side-wall for tests 3, 4 and 6.

4.2 FE model predictions from measurements

As an alternative to the approach described for the blind-prediction study above, the measured pressure-time histories from the 34 experiments summarized in tables 1 and 2 can be applied directly as input to the FE model. Figure 11 illustrates how the data from the eight internal pressure sensors (P1-P8) can be averaged in pairs for test 21: P12 (average of P1 & P2), P34 (average P3 & P4), P65 (average of P5 & P6) and P78 (average of P7 & P8). To minimise the uncertainty associated with permanent deformation of the containers, the analysis focused on tests 1, 21 and 29 (configurations described in tables 1 and 2). Figures 12, 13 and 14 summarise the dynamic response for tests 1, 21 and 29, respectively.

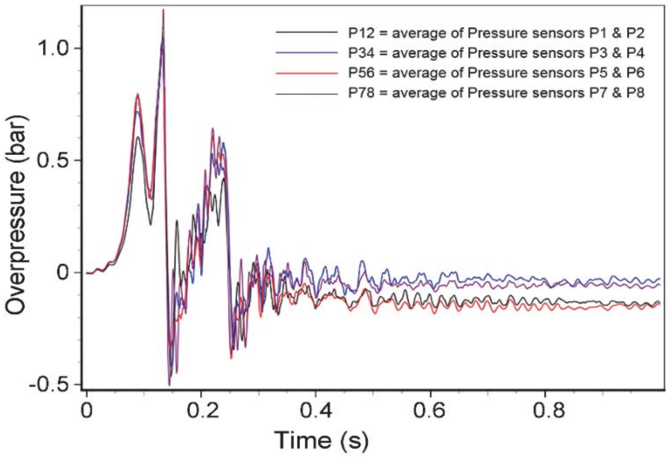
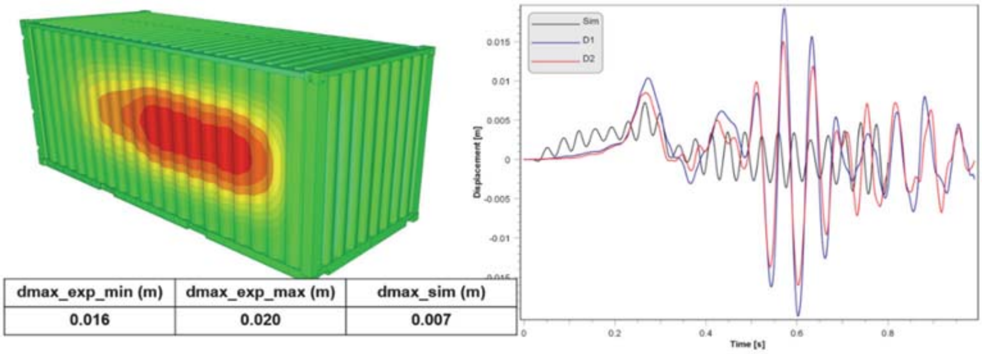
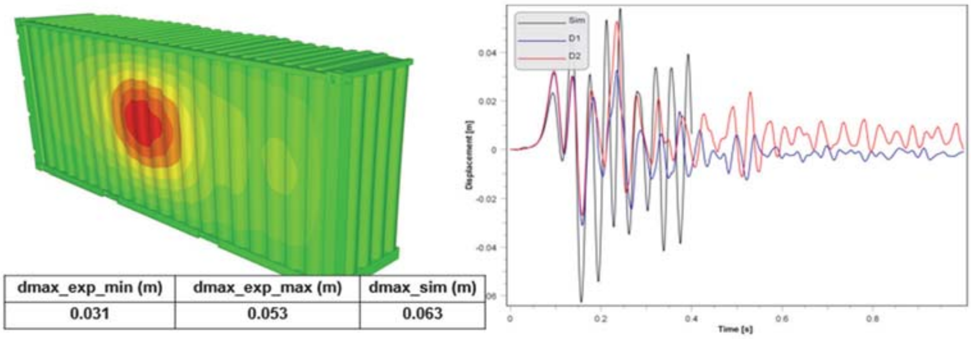


Figure 11 : FE model input from measured pressure-time profiles for test 21.



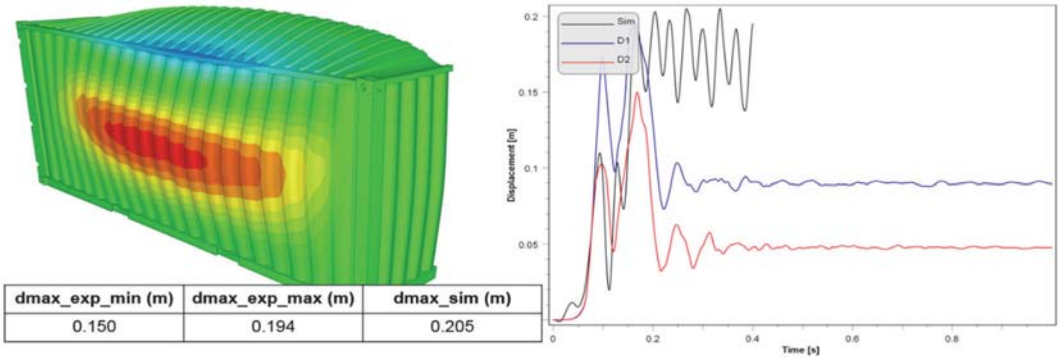
dmax_exp_min (m)	dmax_exp_max (m)	dmax_sim (m)
0.016	0.020	0.007

Figure 12: Displacement-time profiles for test 1.



dmax_exp_min (m)	dmax_exp_max (m)	dmax_sim (m)
0.031	0.053	0.063

Figure 13: Displacement-time profiles for test 21.



dmax_exp_min (m)	dmax_exp_max (m)	dmax_sim (m)
0.150	0.194	0.205

Figure 14: Displacement-time profiles for test 29.

With this approach, the maximum displacement predicted by the FE solver for test 1 is 7 mm, which is significantly lower than the experimental values for tests 1, 2 and 5 (repeated tests): 20, 20 and 42 mm. For test 21, with 21 vol.% hydrogen and venting through a 6.0 m^2 opening in the roof, covered by a 0.2 mm polyethylene film, the predicted maximum displacement is 63 mm, which is comparable to the measured value of 53 mm. For test 29, with 24 vol.% hydrogen, the pipe rack obstacle in position 2 (P2) and venting through a 4.0 m^2 opening in the roof, the FE models predicts a maximum deflection of 205 mm, which compares reasonably well with the measured value of 194 mm. The displacement contours for the sidewalls predict a significantly wider deformation zone, compared to test 21.

Figure 15 summarizes the experimental results and the corresponding model predictions for the tests that included structural response measurements (wall displacement was not measured for tests 9 and 34). In general, the model tends to over-predict the maximum wall deflection, especially for the tests with venting through the doors (tests 1-14). However, given the uncertainties associated with material properties, mapping of discrete pressure data to surfaces, permanent deformation of structures, etc., the model predictions are in reasonable agreement with the experimental values. Repetitive use of the same containers in the test program leads to cyclic plastic deformation and reloading of the materials. This introduces further uncertainties, such as the formation of local buckling and development of kinematic hardening of the material. The FE simulations did not account for any of these phenomena.

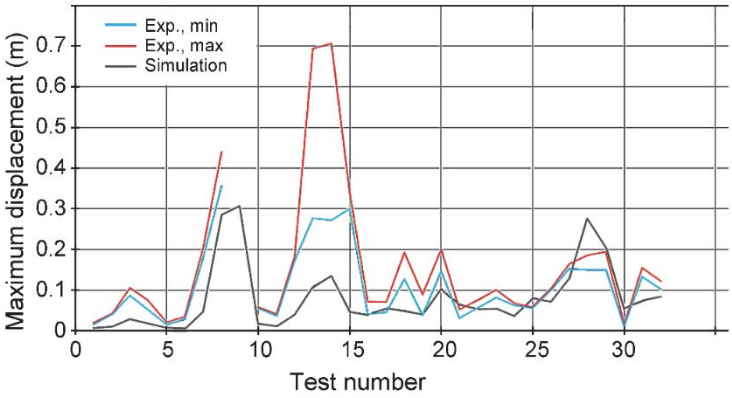


Figure 15: Maximum displacement of side walls for the 34 experiments.

4.3 FLACS-Hydrogen predictions

Figure 12 presents results from CFD simulations of tests 15 and 29 with FLACS v10.5, as well as an in-house development version of FLACS (FLACS β). Figures 17 and 18 show the corresponding pressure-time histories. Both versions of FLACS tend to predict conservative values for the maximum overpressures in enclosures with obstacles (test 29) and without obstacles (test 15). The pressure-time histories are predicted with reasonable accuracy, given the limited repetability for this type of experiments [2-3]. As part of future work in the HySEA project, similar pressure-time data will be used as input to the IMPETUS Afea FE simulator.

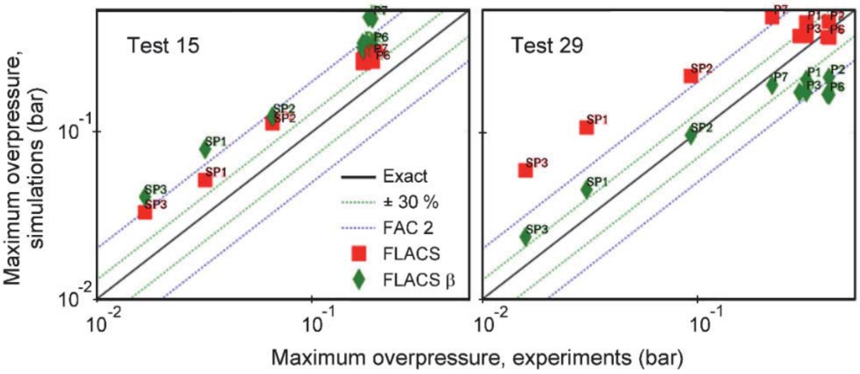


Figure 16: Scatter plot of maximum overpressure for texts 15 and 29.

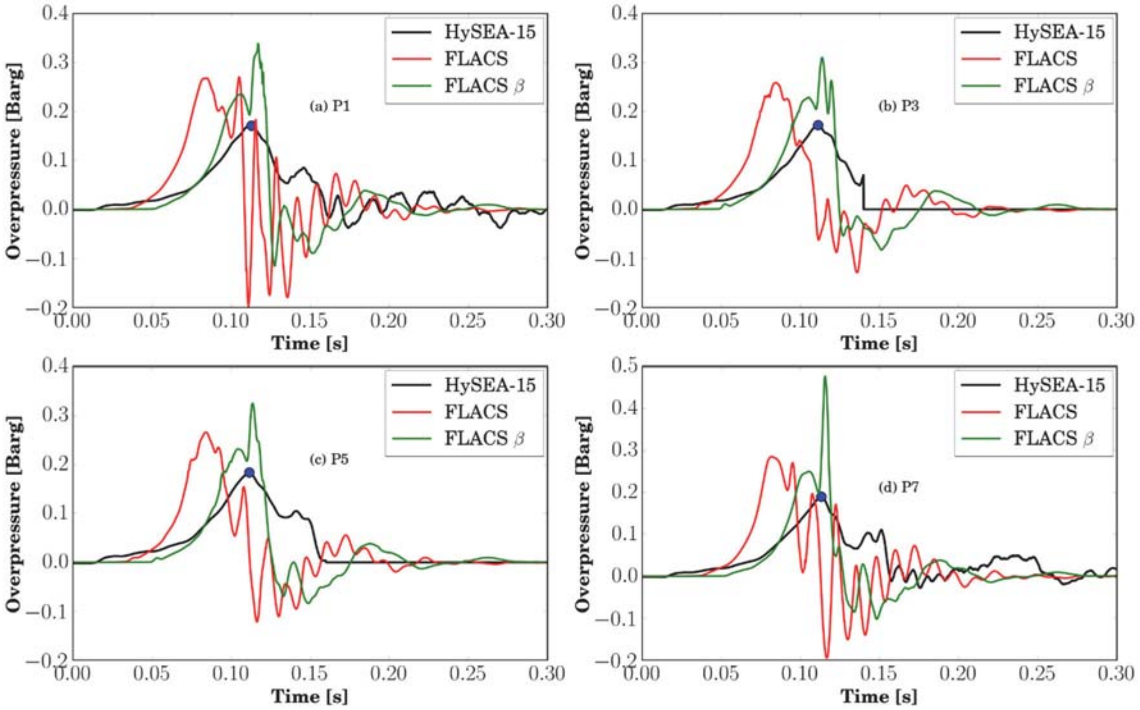


Figure 17: Pressure-time histories for test 15 in positions P1, P3, P5 and P7.

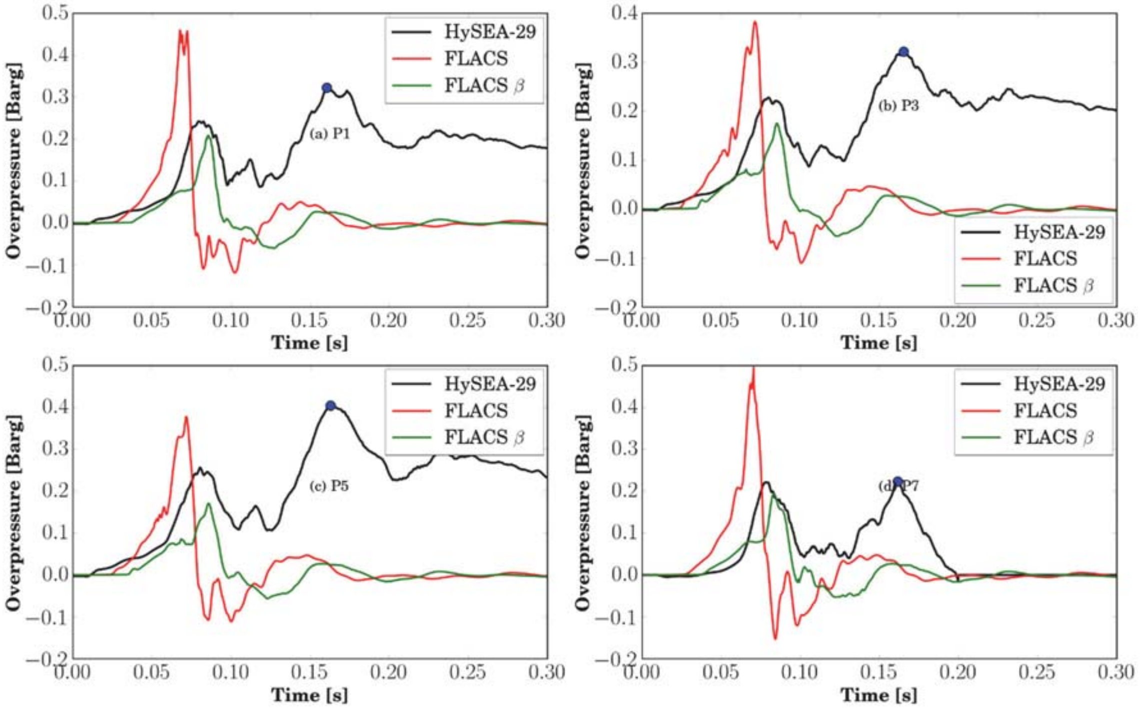


Figure 18: Pressure-time profiles for test 29 in positions P1, P3, P5 and P7.

5. CONCLUSIONS AND FURTHER WORK

The combined CFD-FE model predictions for the structural response of 20-foot ISO containers during vented hydrogen deflagrations are in reasonable agreement with experimental data, except for scenarios where the explosion vessels were severely damaged. This demonstrates that the proposed methodology is viable, provided it can be demonstrated that CFD tools are able to simulate vented hydrogen deflagrations in complex geometries with sufficient accuracy.

Future work in the HySEA project will focus on improving and validating the models for turbulent reacting flow in FLACS-Hydrogen, and refining the integration between the CFD tool and the FE solver. Material properties for the ISO containers will be measured, and the results may contribute to a more accurate geometry model for 20-foot ISO containers in the IMPETUS Afea solver. Finally, the model system will be used to derive pressure-impulse (P-I) diagrams for containers.

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