MODELLING OF H2 DISPERSION AND COMBUSTION PHENOMENA USING CFD CODES

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ABSTRACT

Computational Fluid Dynamics codes are increasingly being considered for safety assessment demonstrations in many industrial fields as tools to model accidental phenomena and to design mitigation (risk reducing) systems. Thus, they naturally complement experimental programmes which may be expensive to run or difficult to set up. However, to trust numerical simulations, the validity of the codes must be firmly established, and a certain number of error sources (user effect, modelling errors, discretization errors, etc) reduced to the minimum. Code validation and establishment of “best practice guidelines” in the application of simulation tools to hydrogen safety assessment are some of the objectives pursued by the HYSAFE Network of Excellence. This paper will contribute to these goals by describing some of the validation efforts that CEA is making in the areas of release, dispersion, combustion and mitigation, thereby proposing the outline of a validation matrix for hydrogen safety problems.

1. INTRODUCTION

Computational Fluid Dynamics (CFD) is a powerful tool that has now found its way into many industrial fields, from aeronautics to automobile, power and chemical industries. CFD is used for design and performance enhancement, and a high level of confidence can generally be attached to such calculations, for the following two reasons:

- CFD codes benefit from a very complete and thorough validation for flows that are representative of the aforementioned industrial applications;
- An increasing awareness of so-called “best practice guidelines” (BPG) [1,2] in setting up and conducting CFD calculations.

In the area of industrial safety, and in particular gas dispersion and explosion issues, the use of CFD is not so advanced. Besides the issue of BPG which can probably be generalised to such applications (the current version of the ERCOFTAC BPG does not deal with multi-component reactive flows), the issue of validation is a crucial matter. It has to rely on experimental data representative of “real size” accidents, which by definition are expensive and technically difficult to conduct. Thus, in general, commercial or academic CFD codes are not validated for such applications, and only dedicated tools have benefited from an extensive validation. This is particularly true for the gas industry, with codes such as ADREA-HF [3], AUTO-REAGAS [4] or FLACS [5], or the nuclear industry with hydrogen risk analysis tools GASFLOW [6], GOTHIC [7] or TONUS [8].

Today, in the field of hydrogen fuel safety, the predictive qualities of CFD codes are not firmly established, and even open benchmark exercises such as conducted recently in the HYSAFE project are characterized by a large scatter of results. It is one of the objectives of the HYSAFE Network of Excellence (NoE) to share hydrogen-risk relevant experimental data among industry, research and regulatory organisations and universities, and to improve the modelling and the validation of the tools to be used in the future for risk assessment studies, and for improving the design and the safety of hydrogen systems. This paper contributes to this objective by reporting on some of the validation exercises that CEA has performed in the area of hydrogen release and dispersion and combustion. Some of this work is performed within benchmark exercises between HYSAFE partners, which are also reported in this conference. Complementary to these validation test cases, we describe additional cases such as transient buoyant flow releases in large scale confined volumes, and hydrogen deflagration or detonations in confined geometries. Hydrogen risk mitigation systems can also be modelled by CFD and we report on the catalytic recombiner experiments performed in the KALI facility of CEA, with the associated numerical simulations. In each case, we describe briefly the physical and numerical models used, and discuss the extent of the validation and the limitation of the models.

2. DISPERSION AND COMBUSTION PHENOMENA

Accidents involving hydrogen usually involve the following phenomena:

- Release of hydrogen, whether in gaseous or liquid form, from a storage system or a distribution system. This release can be characterized by low or high momentum;
- Dispersion into the environment, whether confined, semi-confined or open atmospheres: this process can be diffusion dominated, or convection dominated, or both, depending on flow speeds, level of turbulence, etc.

In the event of a combustible gas mixture being formed, ignition may occur, leading to various combustion modes, which depend on mixture composition, concentration levels, geometrical features such as obstacles or vents, and flow field characteristics such as turbulence,

- Diffusion flames;
- Jet fires;
- Slow deflagrations;
- Flame acceleration leading to fast deflagrations or Deflagration to Detonation Transition (DDT);
- Detonations.

The above phenomena represent a very large range of flow regimes involving chemical and heat transfer processes, from nearly incompressible buoyant flow to fully compressible reactive flow. Simulating them can require very different types of physical models – from simplified engineering correlations to sophisticated chemical reaction and turbulence models. In addition, a very wide range of length and time scales are involved, which, to solve efficiently and accurately, may require different types of numerical schemes and algorithms [8]. Although today state-of-the-art commercial CFD codes may claim to model most of the above phenomena, in-house codes are still quite often used. This is the case for one of the codes that CEA is using, the CAST3M code, which is a structural mechanics, fluid dynamics and heat transfer platform [9], in which specific hydrogen-related models have been developed over the past ten years, whether for nuclear fission reactors (TONUS application developed with IRSN [8]) or other applications such as fusion reactors or hydrogen-energy systems [10,11]. The description of the different physical and numerical models developed to simulate hydrogen dispersion and combustion phenomena is beyond the scope of this paper, but can be found in the following references:

- Low Mach number Finite Element algorithms to describe buoyant flows [12]
- Unstructured 2^{nd} order Finite Volume Riemann solvers to model detonation [13,14];
- Simplified hydrodynamic and combustion model for turbulent deflagrations [15,16];
- Laminar (global Arrhenius rate) and turbulent (Eddy Break-Up) combustion models [17].

In addition to the CAST3M code, CEA is using other codes to model specific phenomena, such as free surface flow characterizing the spill of liquid hydrogen. Use of other codes with more sophisticated features than those currently available in the CAST3M environment is also contemplated in the framework of the HYSAFE project. In the following sections, the current status of the validation of the aforementioned models and methods is discussed through the description of various test cases, including dispersion, combustion and mitigation experiments.

3. DISPERSION MODEL VALIDATIONS

Dispersion model validation is an on-going task in HYSAFE. Two benchmarks in particular have been selected during the first year of the project, the NASA-6 experiment [18] which deals with the liquid spill of H2 followed by evaporation and atmospheric dispersion, and the RUSSIAN-2 experiment [19] which is the mixing of H2 and air in a confined vessel. The former is still on-going and will not be reported here. The latter is discussed here, together with other validation cases dealing with release and distribution in confined atmospheres. In most cases, and for reasons of safety, helium was used in the experiments to simulate hydrogen. This is acceptable given the relative large scale of the experiments, so that buoyancy effects can develop, and also for code validation purposes. Comparison of helium and hydrogen behaviour on the same experimental set-up would however be of interest to fully close the issue of the appropriateness of using helium to simulate hydrogen.

3.1 Russian-2 test

This test [19] was chosen as one of the first benchmark exercises in the HYSAFE project, and it is one of the few experiments known to the authors where hydrogen was actually used. It consists of a steel cylindrical vessel, 5.5m high, 2.2 m diameter, corresponding to a volume of 20m3. Hydrogen is released 1.4m from the top, on the axis of symmetry, at a rate of 4.5l/s, over a period of 60s, and then the injection is stopped and diffusion-dominated mixing takes place over a period of 250min. Unfortunately, the experiment was not repeated and there is very little information about the experimental uncertainty of the data. From a computational point of view, the challenges lie in the short high momentum injection of H2 (turbulence), followed by a very long transient (issue of implicit schemes, time-step, mass conservation of H2, etc). CEA simulated this experiment using the CAST3M code, with an axi-symmetrical Finite Element Low Mach number flow formulation. A mixing length model was used for turbulence, and slip conditions applied at the wall. Fig. 1 shows the H2 concentration isolines for different times, showing the diffusion-dominated mixing process once the injection has been stopped, and a comparison with experimental results. Fig. 2 shows a grid sensitivity study for this test case, which shows that use of too coarse grids can lead to grid-dependent results.

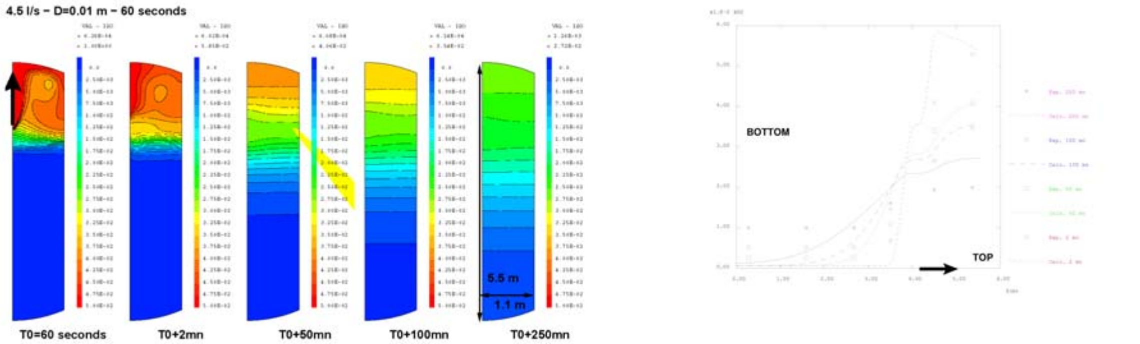

Figure 1: (left) H2 concentration isolines at different times, showing a diffusion-dominated mixing process once the injection is stopped; (right) Comparison between predicted and measured values.

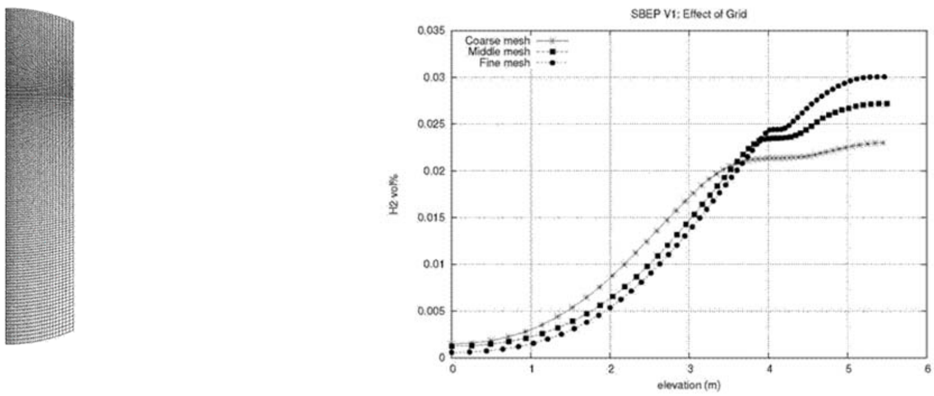

Figure 2: Example of grid used (Medium grid of 7400 nodes), and grid sensitivity analysis of the results, based on a series of grids with a refinement factor of 2 in each direction.

As with most other benchmark computations of this test, our numerical results under-predict the diffusion process. However, our results are within the main stream of the computed results, with an underestimation of the time-evolution of hydrogen enrichment in the lower part of the vessel. The flat profiles that are observed close to the injection level are due to the presence of the injection pipe in the grid. One possible reason for the under-prediction of the diffusion process is that natural convection movements due to possible heat-up of the structures during the injection – neglected in the numerical simulations - may play a role. This hypothesis can unfortunately not be checked since no information on wall temperature is available.

3.2 AECL LSGMF tests

This experiment [20] was performed to study the dynamic of a jet release of helium, simulating hydrogen, in a large scale volume of about 1000m3, depicted in Fig. 3. This experiment is particularly interesting because of the scale of the room in which the release takes place, and because it is three-dimensional. The injection, characterized by a 3 g/s release at a speed of about 8.6m/s during 600s, took place in the centre of the room, near the bottom, and an instrumental grid above the injection point enabled gas concentration measurements. Fig. 4 shows some of the results that were obtained with the CAST3M code (Finite Element formulation for Low Mach number flow), with comparisons with experimental data shown on the right.

Figure 3: AECL Large Scale Gas Mixing Facility

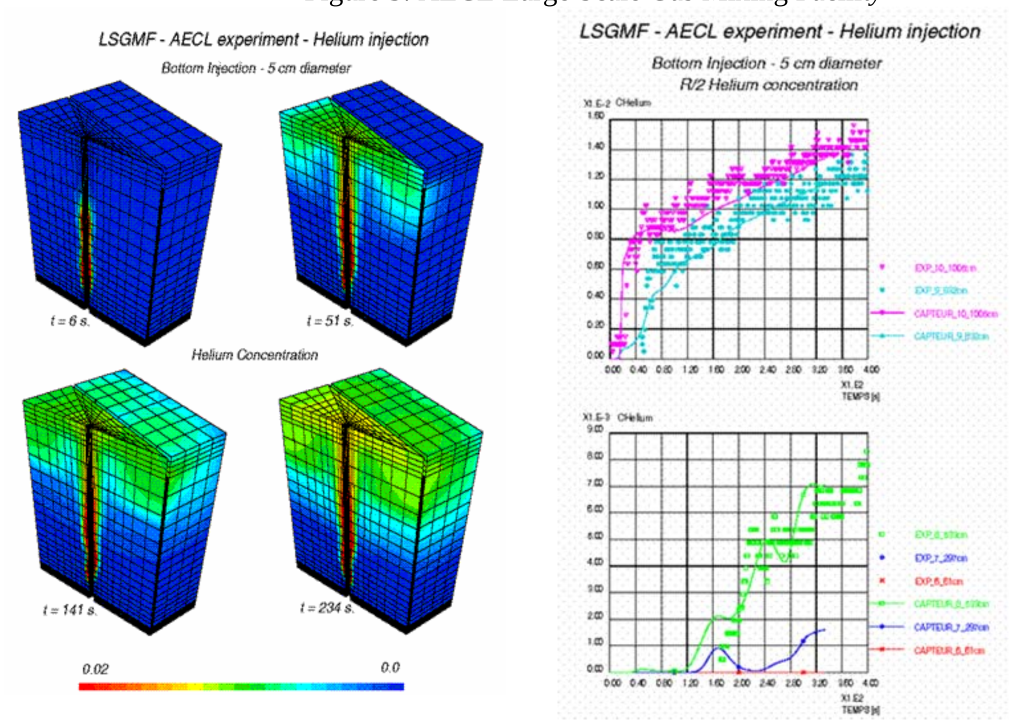

Figure 4: CAST3M simulations: on the left, Helium concentration isolines as different times, and on the right, comparison between computed results and experimental data

Both standard k-ε and RNG-k-ε models were tested, and a better agreement with experimental data was obtained with the latter. The same conclusion was also drawn by Heitsch, with the CFX code [21].

3.3 MISTRA MH1-MH2 tests

MISTRA is a cylindrical steel vessel facility (see Fig. 5), designed for the study of hydrogen risk in the framework of severe accidents for Pressurized Water Reactor plants [22]. Since it is well instrumented relative to its large scale (height 7m, diameter 4m, volume 100m3), and with particular attention paid to the control of the experimental test conditions such as initial and boundary conditions, it is also well suited to the experimental study of H2 release in confined volumes, whether in the form of jets or plumes. Tests (with helium) were performed in 2004 as a basis for future code benchmarking within the HYSAFE project. The MH1 (off-centered injection) and MH2 (centered injection) tests were both characterized by the injection of helium at a mass flow rate of 1g/s through a 75mm diameter nozzle, at ambient temperature and for a duration of 1800s. Concentration measurements were continued for a further 5200s, to follow the diffusion-dominated mixing process. Fig. 6 shows the time-evolution of the helium concentration in different sensor locations, and the way the stratification, with concentration levels near 12% at the top of the facility, is only very slowly broken up by diffusion processes. Preliminary computations of the MH2 test were made using an axi-symmetrical model of the facility. Turbulence was modelled using a mixing length approach, with mixing length based on the diameter of the injection nozzle. This is well suited to the modelling of the buoyant jet, as seen in the comparison between the predicted axial velocity profile and Laser Doppler Velocimetry (LDV) measurements at different times during the injection (Fig. 7). There is also a satisfactory agreement between predicted concentration profiles and experimental values – though improvements can probably be made by adjusting turbulence parameters (especially for the predictions in the bottom of the facility, where the discrepancy is the most noticeable), and after having performed grid and time-step sensitivity studies. In many aspects, this experiment is very close to the Russian-2 experiment. However, we think the data is of better quality, because each test has been repeated, and temperature measurements for the structures are available. This may help close the issue associated with the “natural convection” mixing identified in the HYSAFE benchmark problem.

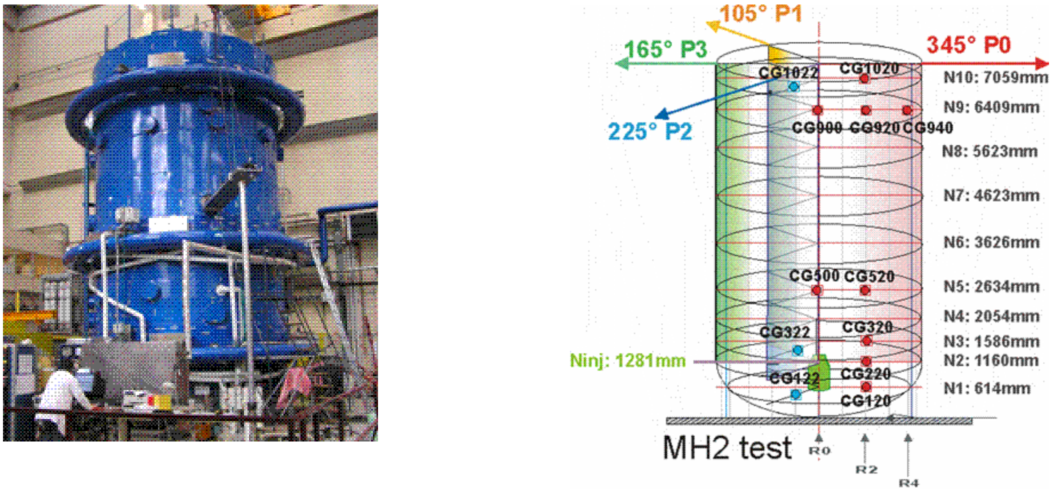

Figure 5: View of the MISTRA facility and position of sensors for the MH1 (and MH2) tests

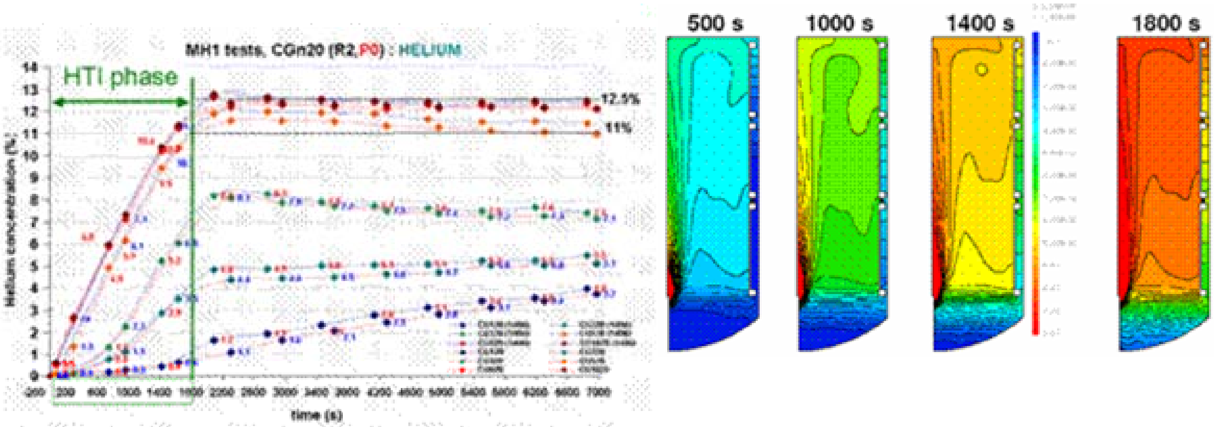

Figure 6: (left) Measured concentrations in the different sensor locations as a function of time; (right) Predicted He concentration contours at different times during the injection;

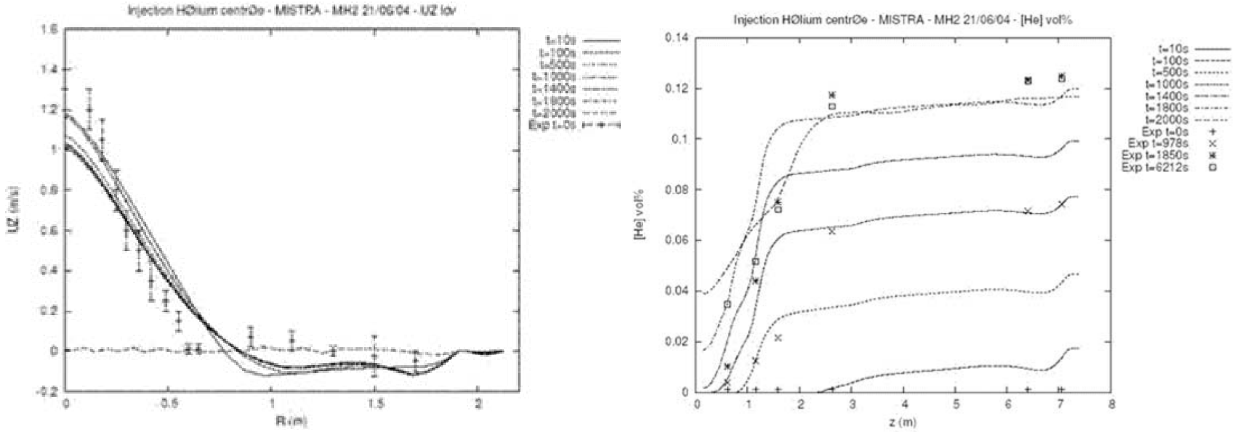

Figure 7: (left) Comparison of predicted axial velocity and LDV measurements; (right) Comparison of predicted and measured He concentration at different times along the vertical axis.

4. COMBUSTION MODEL VALIDATION

CEA has validated its combustion models [13,15,16,17] implemented in the CAST3M code on different “large scale” confined experiments. The CREBCOM model was also recently applied to the Fh-ICT H2 Balloon experiment (atmospheric deflagration of a 20m diameter hemi-sphere filled with stoichiometric mixture of air and hydrogen), in the framework of an HYSAFE benchmark. The simulation results are not reported here due to lack of space. We focus here on flame propagation experiments in confined geometries, starting from slow flames up to fast turbulent deflagration and detonations (DDT phenomena are not resolved in the CAST3M code).

4.1 HDR E12.3.2 Test

This experiment, carried out in the HDR containment in Germany [23] consists in a “slow” hydrogen deflagration in a series of interconnected comparments, as shown in Fig. 8 and Fig. 9.

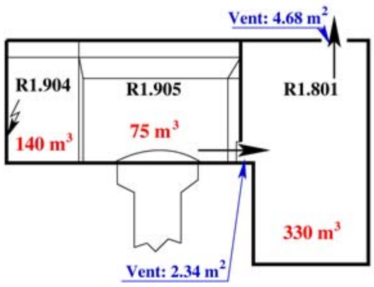

Figure 8: HDR test E12.3.2. Sketch of the problem.

The initial gas mixture composition is: 10 % vol of hydrogen, 25 % vol of steam and 65 % vol of air at the pressure of 1 bar and the temperature of 337 K. Ignition takes place at the far end of the room R1.904. During the experiment the following phenomena were examined:

- flame propagation in the compartments;
- flame front acceleration at the vent and its effect on the pressure increase.

During the experiments it was found that the accelerated jet ignition results in the highest peak pressure of 1.3 bar. The experiment was modelled using the CAST3M code and the CREBCOM combustion model. The 3D geometry of the test with location of the probes is shown in Fig. 8.

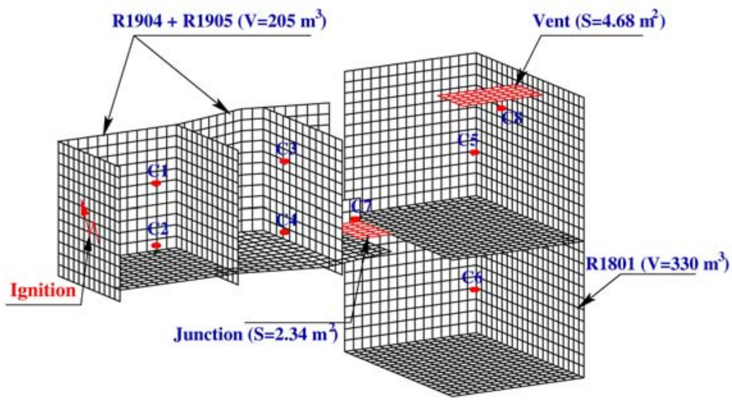

Figure 9: Geometry of the problem with probes positioning.

The parameters of the CREBCOM model were chosen by trial and error so as to get a good agreement between the numerical results and the experimental values of pressure, as shown in Fig. 10 (left). But it has to be emphasized that these results are grid-dependent: on a finer mesh, with the combustion parameters left constant, a shift in time is observed compared to the coarse mesh results.

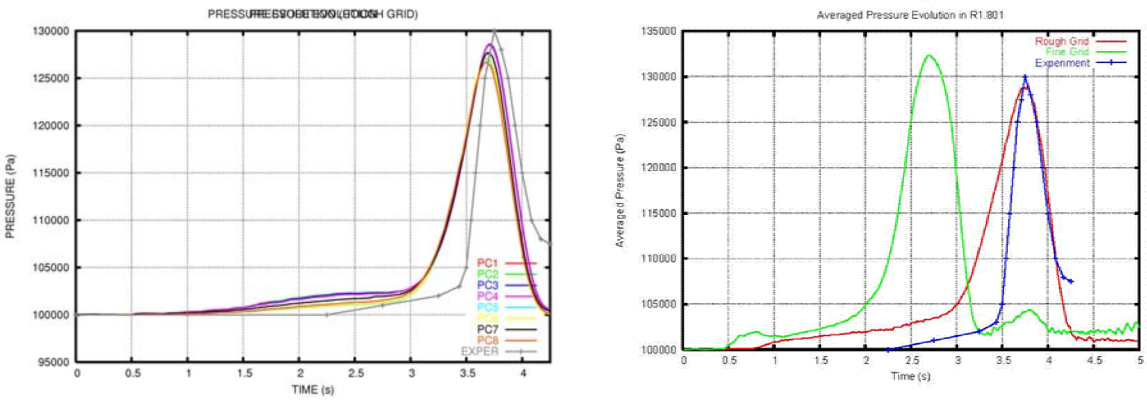

Figure 10: Computed pressure vs. data. Left, coarse mesh results. Right, effect of grid refinement

The qualitative results for the coarse mesh are presented in Fig. 11. They clearly show the jet ignition phenomenon. We can observe the abrupt change in the flame velocity when it enters the room R1.801. The hydrogen gas in the larger room R1.801 is almost completely burned within 0.5 s.

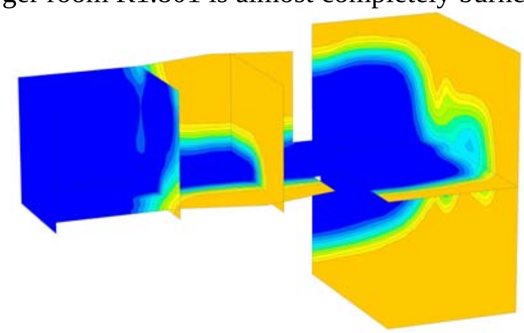

Figure 11: The hydrogen mass fraction at t=3.4 s.

4.3 BATTELLE BMC Ex29 Test

Test BMC Ex29 is another large scale deflagration experiment, carried out in the Battelle Model Containment [24]. The geometry (Fig. 12) consists of two compartments R7 and R5 of 41 m3 each, separated by a vent of 1.4 m2 (blockage ratio = 66 %). In room R7, there is an obstacle (cylinder) of the blockage ration 50 %. At the far end of room R5, there is a vent of surface area 1.8 m2.

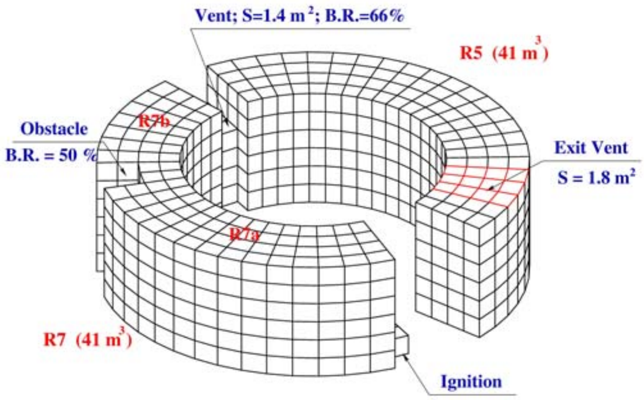

Figure 12: BMC test Ex29. Geometry

The initial gas composition mixture is 10 % vol. of hydrogen and 90 % vol. of air at atmospheric pressure and the temperature of 337 K. Ignition takes place at the far end of room R7, then the flame accelerates after passing the cylindrical obstacle. The highest peak pressure of 1.9 bar is reached soon after the flame enters room R5. The CREBCOM model was used to model the deflagration, with its parameters chosen so as to get a good agreement for pressure evolution between the numerical results and the experimental values, as shown in Fig. 13. As with the HDR test, results have been found to be grid sensitive.

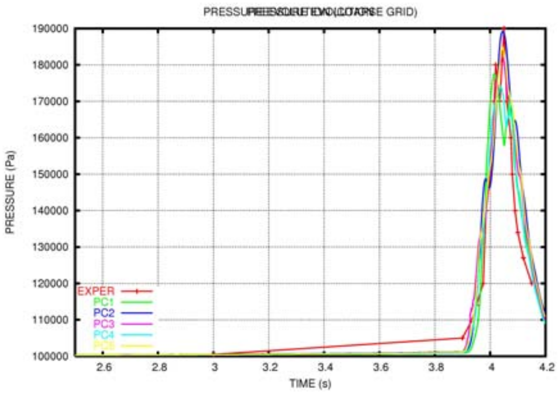

Figure 13: Pressure histories. The red line corresponds to the experimental results.

The qualitative results are presented in Fig. 14. The major pressure increase happens when the flame enters the room R5 which is in a good agreement with experimental results.

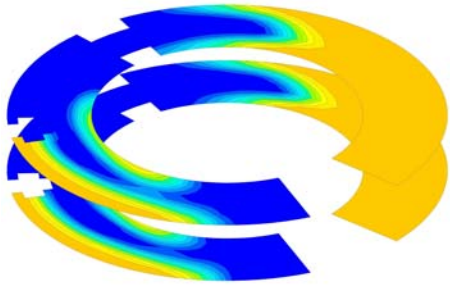

Figure 14: hydrogen mass fraction isolines at t=3.95 s.

4.4 RUT STH06 Test

The RUT facility of the Kurchatov Institute [25] is a 480m3 reinforced concrete building with two channels and a large central compartment called canyon. The first channel is over 36m long, 2.5m wide and 2.3m high. Obstacles are located in this channel so as to enhance turbulence and thus accelerate the flame. The channel opens into the upper part of the canyon which is 10m long and 6.3m deep, and then onto the second channel, which is curved. Test STH06 is a fast deflagration experiment, with 16.2% H2, 38.8% air and 45% steam as initial conditions. A two-dimensional simulation was performed, using the CREBCOM model with adjusted parameters for this fast deflagration case. The reflected shock waves are clearly present as seen in Fig. 15. The comparison with experimental data is also satisfactory, although use of finer meshes would be needed to capture the pressure peaks better (but the mesh sensitivity in terms of flame front propagation is less pronounced than for slow deflagrations).

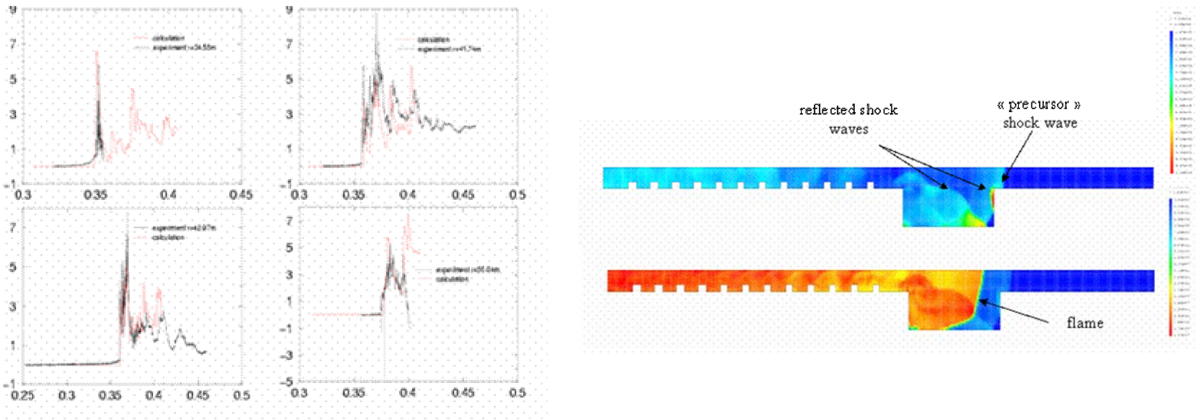

Figure 15: STH06 Fast deflagration calculation: on the left, comparison between predicted values and experimental measurements, on the right, pressure and temperature isolines (from [16])

4.5 RUT STM4 Test

The CAST3M code was also validated on a fully developed detonation test performed in the large scale RUT facility. In test STM4 [25], a homogeneous mixture of air, steam and hydrogen corresponding to a (dry) concentration of 24.8%, at atmospheric pressure and 90oC. The mixture was ignited at the beginning of the first channel and transition (which was not modelled) occurred before the end, so that a fully developed detonation wave entered the canyon. It is this part of the flow that was modelled, using the compressible flow solver of CAST3M (2^{nd} order unstructured Finite Volume method with Flux Vector Splitting for the Euler fluxes, and a one-step global Arrhenius reaction rate [13]. Several meshes were considered, to assess grid dependency of the results. The finest mesh used had nearly 30000 cells. Figure 16 shows a good agreement between experiment and simulation.

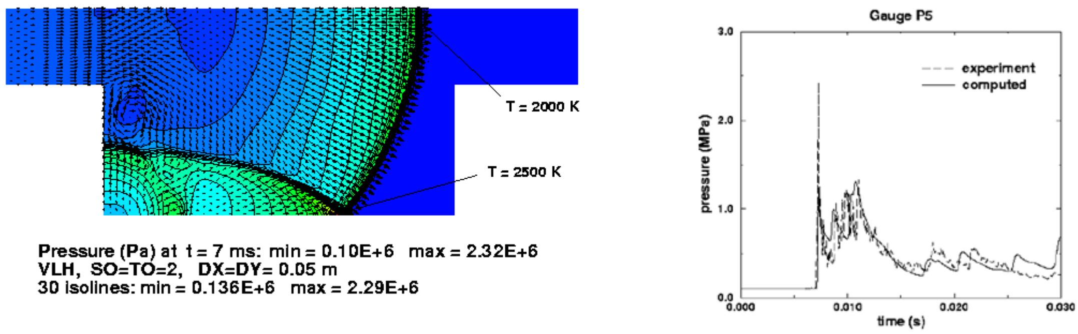

Figure 16: On the left, pressure isolines from the CAST3M two-dimensional plane calculation, and on the right, comparison between computed results and pressure measurements.

5. MITIGATION MODEL VALIDATION

Mitigation systems include both risk-reducing measures and consequence-reducing measures. We report here one experiment, which deals with a risk-reducing system, passive auto-catalytic recombiners (PARS). PARS are systems which help reduce hydrogen content in an atmosphere by consuming hydrogen on catalytic surfaces, and therefore can help mitigate the risk of explosion by maintaining the concentration levels below flammability limits. Such systems are installed for example in the containments of Pressurized Water Reactors (PWR) to control hydrogen risk in the event of a severe accident. Catalytic burners are also considered for hydrogen-powered vehicles to control the amount of hydrogen released in case of boil-off. CFD modelling of hydrogen release and mixing, taking into account the effect of a recombiner system can help to improve the performance of the mitigation device, for example by locating it in the most appropriate position.

The test case reported here deals with one of the many recombiner tests performed in the KALI facility of CEA [26], and has been used to validate the recombiner model implemented in the CAST3M code (and in particular, in the TONUS application developed for IRSN [8,16]). This facility is a 15.6m3 steel facility equipped with various injection systems, where a recombiner casing with its catalytic plates can be installed. During the test, global hydrogen concentration measurements were made. Figure 17 shows the temperature contours of a CFD calculation, where the thermal plume (hot combustion gases) exiting from the recombiner casing is clearly visible. Unfortunately, no experimental data is available to validate the predicted flow field. The calculated time-evolution of hydrogen concentration is in good agreement with the experimental data.

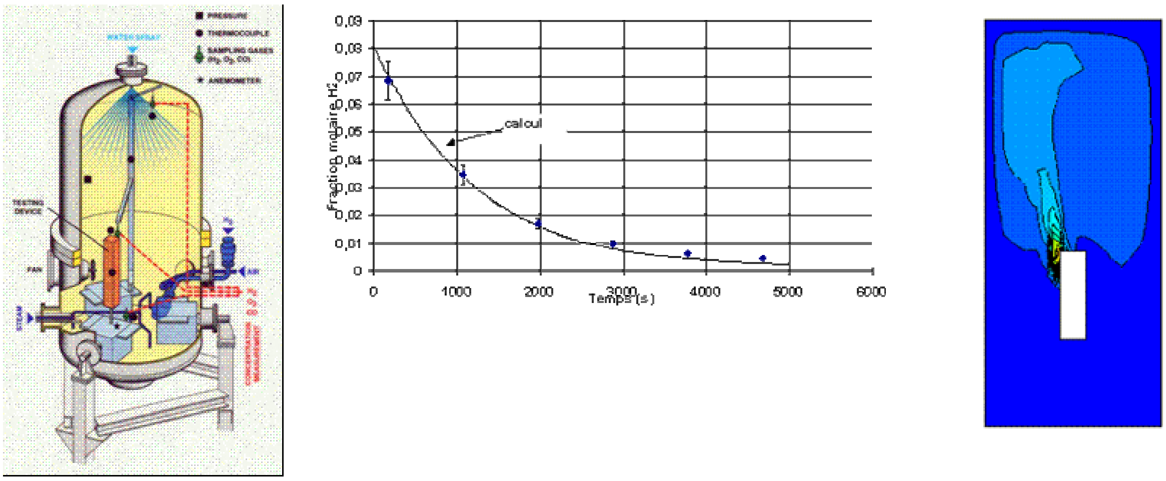

Figure 17: From left to right, diagram of the KALI facility of CEA, numerical predictions vs. experimental measurements of global hydrogen concentration as a function of time, and temperature contours showing the thermal plume exiting from the recombiner outlet.

6. OUTLINE OF A VALIDATION MATRIX – GAPS AND STANDING ISSUES

We have reported on a series of test cases covering release, dispersion, combustion and mitigation in open or confined environments, on which CEA has validated or is currently validating its computational tools. This “matrix” (see table 1) is by no means complete, as many phenomena are still to be addressed, and for those that are addressed, the quality of the data is not always sufficient for code validation purposes so that new experiments are required. Also, in many cases, more systematic sensitivity analyses (grids, model parameters, numerical parameters) and application of BPG are needed, in order to conclude. However, we think that this table could form the basis of a widely-agreed validation matrix for the application of CFD codes to hydrogen safety problems.

Current identified gaps in terms of the validation of CEA’s CAST3M code are the following:

- low momentum release in confined atmospheres
- atmospheric dispersion (on-going in the framework of the NASA-6 benchmark, together with the modelling of the LH2 spill)
- combustion in the presence of gradients
- diffusion flames and jet fires.

Table 1. Outline of CEA's CAST3M code validation matrix for H2 safety – relevant phenomena

Name of experiment	Media	Geometry, Scale	Open, semi-confined or confined atmosphere	Main phenomena	Quality of experimental data (High – Medium - Low)	Features of validation
RUSSIAN-2	GH2	Cylindrical vessel, 5.5m high, 2.2m diameter, **20m3 vol.**	confined	Subsonic release near the top at a rate of 4.5l/s for 60s, then diffusion over a period of 250min	Low	grid-dependence
AECL LSGMF	GHe	Rectangular room, **1000m3**	Confined	Buoyant jet release of 3g/s at a speed of 8.6m/s for 600s	High	turbulence model
MISTRA MH1-MH2	GHe	Cylindrical vessel, 7m high, 4m diameter, **100m3**	Confined	Buoyant jet release of 1 g/s for 1800s, then diffusion over a period of 7000s	High	Preliminary calculations
NASA-6	LH2	**40m**	Open, non congested	spill of LH2, evaporation, heat transfer ground, atmospheric dispersion, buoyancy forces	Medium	On-going (coupling FLUENT-CAST3M codes)
Fh-ICT Balloon	GH2	**80m**	Open, non congested	Deflagration of a 20m diameter half-sphere and propagation of pressure waves over a distance of 80m	Medium	model parameters, grid dependence
HDR E12.3.2	GH2 + steam	Series of interconnected rooms of respective volumes **140m3, 75m3 and 330m3**	Semi-confined (last room vented)	Ignition at far end of a hydrogen, steam and air mixture followed by flame propagation (deflagration) and acceleration	Low (designed for lumped-parameter codes)	model parameters, grid dependence
BATTELLE BMC Ex29	GH2	Series of two interconnected rooms of **41m3** vol. each	Semi-confined (second room vented)	Ignition at far end followed by flame propagation (deflagration) and acceleration	Low (same reason as above)	model parameters, grid dependence
RUT STH06	GH2	Two long channels (about 36m each) separated by large vol. (canyon), overall volume **480m3**	Confined	Fast deflagration	High	grid dependence
RUT STM4	GH2 + steam	Same as above	Confined	Fully developed detonation entering the canyon	High	grid dependence, order schemes
KALI	GH2 + steam	Steel vessel of **15.6m3**	Confined	Global H2 reduction through the use of a Passive Autocatalytic Recombiner	Low	None

8. CONCLUSIONS

A series of release, dispersion and combustion experiments that have been used or are being used by CEA to validate its CFD tools, and which could form the basis of a broadly recognized validation matrix, has been described. This work is still on-going, as in some cases, improvements need to be made to the physical or numerical models. Also, the quality of the experimental data is not always fully satisfactory, so that either more tests need to be performed, or existing test data needs to be made available. The HYSAFE project offers the framework for sharing data and experience, and it is hoped that combined efforts in the field of CFD modelling and validation will lead to more predictive tools and the development of "best practice guidelines" for carrying out numerical simulations of hydrogen accident scenarios in representative environments.

ACKNOWLEDGEMENTS

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