

DEVELOPMENT OF A MODEL EVALUATION PROTOCOL FOR CFD ANALYSIS OF HYDROGEN SAFETY ISSUES – THE SUSANA PROJECT

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ABSTRACT

The “Support to SAfety aNAlYsis of Hydrogen and Fuel Cell Technologies” (SUSANA) project aims to support stakeholders using Computational Fluid Dynamics (CFD) for safety engineering design and assessment of FCH systems and infrastructure through the development of a model evaluation protocol. The protocol covers all aspects of safety assessment modelling using CFD, from release, through dispersion to combustion (self-ignition, fires, deflagrations, detonations, and Deflagration to Detonation Transition - DDT) and not only aims to enable users to evaluate models but to inform them of the state of the art and best practices in numerical modelling. The paper gives an overview of the SUSANA project, including the main stages of the model evaluation protocol and some results from the on-going benchmarking activities.

1.0 INTRODUCTION

Hydrogen safety issues must be addressed in order to ensure that the wide spread deployment and use of hydrogen and fuel cell technologies can occur with the same or lower level of hazard and associated risk compared to conventional fossil fuel technologies. CFD is increasingly used to perform safety analysis of potential accident scenarios related to the production, storage, distribution and of hydrogen and its use in fuel cells. CFD is a powerful numerical tool that can provide useful data and insights but it also requires a high level of competence and knowledge in order to be used in a meaningful way. To apply CFD with a high level of confidence on the accuracy of the simulation results, two main issues have to be addressed: the capability of the CFD models to accurately describe the relevant physical phenomena and the capability of the CFD users to follow the correct modelling strategy.

In this context, a workshop with recognised experts in the field of hydrogen safety was held at the Institute for Energy and Transport of the Joint Research Centre in The Netherlands in order to identify the gaps in CFD modelling and simulation of hydrogen release and combustion. The main outcomes of the workshop were included in a report entitled “Prioritisation of Research and Development for modelling the safe production, storage, delivery and use of hydrogen” [1]. One of the main gaps

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identified was the lack of a Model Evaluation Protocol (MEP) for hydrogen technologies such as the MEP of Ivings et al. [2-3] for LNG technologies.

The SUSANA project (co-funded by the Fuel Cell and Hydrogen Joint Undertaking) aims to meet this need by producing a Model Evaluation Protocol for hydrogen technologies safety (HyMEP) [4]. The project brings together partners with an established track-record in hydrogen safety, along with fundamental and industry-driven CFD research from across Europe. The partners include stakeholders from research organisations (KIT-G, NCSR, JRC), universities (Ulster University - UU), industry (AREVA/HELION, Element Energy), and regulators (HSE/HSL). The project started in September 2013 and will be completed in August 2016.

The CFD Model Evaluation Protocol aims to be the reference document for all CFD users, both to assess their capability of correctly using the codes and to evaluate the accuracy of the CFD models themselves. The Protocol is expected to be beneficial for all the CFD developers (academia and research institutes) and users (like industry and consultancy companies) but also for regulatory/certifying bodies that have to permit hydrogen vehicles and/or hydrogen infrastructure and facilities. Regulatory/certifying bodies will have a document that helps them evaluate whether the CFD analysis supporting permission requests is scientifically sound or meaningless calculation.

The development of the HyMEP builds up on previous experience and projects that were performed for other technologies and applications [5-13].

A Model Evaluation Group (MEG) was established by the European Community in the early 1990s. The group was set up to develop methods for the evaluation of models in the major industrial hazards area because it had become apparent that models used in industrial hazard assessment had never been formally validated. Nevertheless, those models were used as the basis for decisions that directly affected public safety and the environment. In 1994 the group published guidance on model evaluation protocols [5] which provides a framework for the key activities needed to evaluate models: model description, scientific assessment including limits of applicability, user-oriented assessment including ease of use, verification and validation.

Testing the results of model predictions against experimental data, Kakko et al. [6] highlighted the need for suitable databases of model validation data as these were often difficult to obtain or not presented in a way suitable for model validation. A classic example of a model validation database is the modeller's data archive (MDA) of Hanna et al. [7] which recognised the need to collate data in a suitable form in a way that could be accessed by model developers. Since then, some other datasets have been produced, such as the Rediphem database [10].

The SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models) project [11,12] brought together the concept of a model evaluation protocol and specialised database. Its main aim was to provide a methodology not only for validation but also scientific review of models. The project focussed on situations in which complex effects such as aerosols, topography and obstacles were important, as well as simple situations. Ivings et al. [2,3] set out a Model Evaluation Protocol for models used to predict the dispersion of vapours from Liquefied Natural Gas (LNG) installations. The protocol is based upon the SMEDIS project but is not confined to the modelling of LNG spills. One of the recommendations of the MEP by Ivings et al. [2,3] was that validation should be performed by running models against experiments from a validation database that was constructed for this purpose [13].

2.0 THE HYDROGEN MODEL EVALUATION PROTOCOL (HYMEP)

The structure of the HyMEP is illustrated in Figure 1. The initial stage of the HyMEP is the scientific assessment of the model whose purpose is to establish the scientific credibility of a model. In that

stage a preliminary qualitative assessment of the model is performed, by comparing the features of the model (both the physical model and the numerical scheme) with the current state of the art available in the scientific and technical literature. The suitability of the model and of the numerical schemes to completely capture the desired phenomena should be addressed at that stage. The range of applicability of the model, the limitations and advantages of the approach, and any special feature of the model should be identified, according to the available literature and the current common knowledge of the scientific community in the relevant fields. In order to assist the scientific assessment in the field of hydrogen safety technologies, the SUSANA project consortium produced a review of the state-of-the-art in CFD, physical and numerical modelling applied to safety analysis in FCH technologies [14]. Moreover a “Best practices in numerical simulation” guide is in preparation in the project with the purpose of supporting the correct application of CFD models to each relevant phenomenon by the CFD users.

Verification is used to ensure that a mathematical model has been correctly implemented in software i.e. the equations are correctly solved. In validation, model outputs are compared with measurements of physical parameters to demonstrate that the model captures “real world” behaviour across its intended range of applicability. Verification and validation procedures are under development in the project. A database of problems for verification of codes and models against analytical solutions and a Model Validation Database of experiments for validation of simulations covering a range of phenomena relevant to FCH safety are under construction.

How changes in model parameters affect the results is evaluated in the sensitivity study. Model predictions may be sensitive to uncertainties in input data, to the level of rigour employed in modelling relevant physics and chemistry, and to the adequacy of numerical treatments. The sensitivity analysis methodology allows the dominant variables in the models to be highlighted, defining the acceptable range of values for each input variable and therefore informing and cautioning any potential users about the level of care to be taken in selecting inputs and running model. Relevant model parameters include the computational mesh, the time step, the numerical scheme, the boundary conditions, and the domain size for semi-confined, vented and open configurations.

In the statistical analysis of the comparison between experimental data and simulation results, Statistical Performance Measures (SPM) provide a measure of the error and bias in the predictions, i.e. the spread in the predictions such as the level of scatter from the mean and the tendency of a model to over/under-predict. In the validation procedure acceptable numerical ranges for the SPM are going to be defined as quantitative assessment criteria. The key-target variables are identified for each phenomenon that is relevant for hydrogen safety: release, mixing and dispersion, self-ignition, fires, deflagrations, detonations and deflagration to detonation transition. As an example, hydrogen concentration, flammable mass, and velocity can be considered as the first key-target variables for the release and mixing of hydrogen leaking from a tank of a vehicle in a private garage.

The final step in the HyMEP is to prepare an assessment report that includes information and data about each stage of the protocol for the specific model that has been evaluated. In the project the content and the level of details required for the report will be defined.

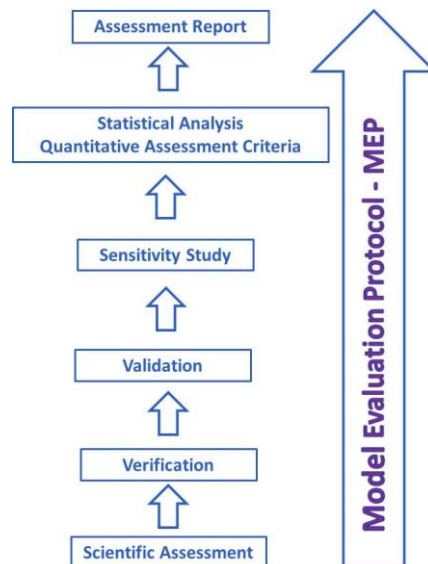


Figure 1. Structure of the Model Evaluation Protocol (HyMEP)

3.0 THE VALIDATION DATABASE

The first version of the model evaluation database is available on the project website [4] and it includes about 30 experiments. The experiments are grouped together according to the relevant phenomena: release and dispersion, ignition, deflagrations, detonations and DDT. Experiments with fires will be added in the next version. A brief description with the experimental set-up and procedure (illustrated by images and drawings where appropriate), the objective of the experiment, the experimental data and references are included for each experiment. In Table 1-5, the lists of experiments that have been identified as suitable for the model validation database in the first part of the project are described for each physical phenomenon.

In the releases and dispersion section, several experiments are available in the database as shown in Table 1. Different relevant configurations are investigated in the selected experiments: indoors and outdoors, small enclosures and garage facilities, and vented configurations. Most of the experiments are performed with gaseous hydrogen (or helium) and only one with liquid hydrogen [21].

In the ignition and fires section only one set of experiments is currently available, as described in

Table 2. The scope of the experiments is to investigate the self-ignition of gaseous hydrogen in a pressurized tube at different pressures with a T shaped pressure relief device [31, 32].

In the deflagration section 14 experiments are available. Some relevant configurations are considered in the experiments: different hydrogen concentrations, an open environment, a closed or vented box, and the presence of obstacles. For example, there are deflagration experiments in the large scale RUT (closed) facility [34], in the obstructed closed and vented tube [34], in a mock-up of a hydrogen refuelling station [38], and in a completely open environment [39,40].

Two sets of experiments of DDT are available in the database. In the first set of experiments DDT with hydrogen in straight pipes of three different diameters and with different gas concentrations are performed [41] while in the second set of experiments explosions in an obstructed 12 m long tube are carried out with a 15% hydrogen-air mixture.

In the detonation section three experiments are included with different hydrogen concentrations: a detonation of stoichiometric hydrogen-air mixture in a hemispherical balloon in open environment [42] and detonations of lean hydrogen-air mixtures (20%, 25%) in a closed large scale facility [43].

In some cases, a report with the experimental data is not directly available. In those cases the reference is to papers where numerical simulations of the experiments are performed and compared to the experimental data.

Table 1: List of release and mixing experiments in the validation database.

Release and Dispersion	
GAMELAN [15,16]	Validation experiments were carried out at CEA in the GAMELAN facility with sizes HxWxL=1.26x0.93x0.93 m with one vent located on a wall. Vents were located at a wall opposite to that where sensors are located. The release of helium was directed vertically upward from a pipe located 21 cm above the centre of the floor. Two different internal diameters of the pipe were considered: 20 mm and 5 mm. Volume fraction of Helium is measured at different positions inside the box.
SBEP_21 [17,18]	The GARAGE facility is representative of a realistic single vehicle private garage. The GARAGE facility is situated indoors to attenuate the variations in meteorological conditions. The internal volume of GARAGE is 40.92 m ³ . Continuous injection of helium is performed in the GARAGE. Volume fractions of the gas are measured at different positions.
GEXCON	Hydrogen gas was released as a jet inside a lab scale facility. The experimental rig consists of a 1.20 m x 0.20 m x 0.90 m vessel, divided into compartments by use of 4 baffle plates with dimensions 0.30 m x 0.20 m. There is one vent opening at the wall opposite the release location centrally located. Different installations of the plates and nozzle diameters are used in the test. Hydrogen concentrations are measured.
INERIS-6C [19, 20]	The experiment INERIS-TEST-6C was performed within the InsHyde project by INERIS, consisting of a 1 g/s vertical hydrogen release for 240 s from an orifice of 20mm diameter into a rectangular room (garage) of dimensions 3.78 X 7.2 X 2.88m in width, length and height respectively. Two small openings at the bottom of the front side of the room assured constant pressure conditions. Hydrogen concentration was detected by 16 sensors.
NASA-6 [21]	The experiments consisted of ground spills of up to 5.7 m ³ of liquid hydrogen (402 kg), with spill durations of approximately 35 seconds. Instrumented towers located downwind of the spill site gathered data on the temperature, hydrogen concentration and turbulence levels.
SBEP_1 [22, 23]	A subsonic release of hydrogen in a closed vessel with height 5.5 m, diameter 2.2 m and volume 20 m ³ . The concentrations of hydrogen are detected by 6 sensors installed at the central line of the vessel.
Swain_GARAGE [24, 25]	The experimental facility represents a full-scale garage with dimensions 6.4 x 3.7 x 2.8 m and two vents on the door. Vent openings with varying height were examined. A full-scale plywood model vehicle was placed inside the garage. The helium flow rate was 7200 l/h and the release lasted for 2 h. Volume fractions of the Helium are measured at different positions.
Swain_HALLWAY [26 -28]	In the vented hallway experiment, the hydrogen leaks from the floor at the left end of a hallway with the dimension of 2.9 m x 0.74 m x 1.22 m. At the right end of the hallway, there are a roof vent and a lower door vent for the gas ventilation. The hydrogen leak is at 2 SCFM (Standard Cubic Feet per Minute) and for a period of 20 minutes.
Release 1 [29]	Hydrogen distribution tests in horizontal free turbulent jet have been carried out in a compartment with an internal volume of 160 m ³ . Experimental facility consisted of high pressure gas system to provide hydrogen release at pressures in the range 20 – 260 bar through the nozzle. Experiments were made in order to evaluate amount of burnable hydrogen – air mixture (above the lower flammability limit) in free turbulent jet at different pressures.
Release 2 [30]	A set of experiments involving horizontal high-pressure hydrogen jet releases was conducted at HSL. Different release pressures and nozzle diameters were used.

Table 2: List of ignition experiments in the validation database.

Ignition		
PRD (Pressure Device) [31, 32]	Relief	High pressure hydrogen gas was released through a T shaped pressure relief devices. In the experiment, the tube was filled with different pressure to investigate the relation between the pressure and self-ignition.

Table 3: List of deflagration experiments in the validation database.

Deflagrations	
HYKA A2 [33]	The experiment was performed in the HYKA A2 experimental facility. A homogeneous mixture of hydrogen (10 vol.%), steam (25 vol.%) and air was established in the vessel. The initial pressure was 1.49 bar, and the average initial temperature was about 90.0 °C. The mixture was ignited at the bottom. Pressure and temperature were measured at different axial and radial locations.
HYCOM-HYC01 HYCOM-HYC12 HYCOM-HYC14[34]	Experiments of hydrogen-air mixture deflagrations were performed in the large scale RUT facility. Different geometry, different ignition positions in the RUT facility and different initial hydrogen concentrations were considered. Pressure data was collected in the experiment.
HYCOM-MC03 HYCOM-MC12 HYCOM-MC43 [34]	Combustion experiments have been carried out in obstructed tube of 174 mm in diameter and 12.2 m in length (DRIVER facility). Ignition at one end of the tube. MC03: 10% Hydrogen/air mixture, blockage ratio=0.6. MC12: 13% Hydrogen/air mixture, blockage ratio=0.6. MC43: in first half of the tube 13% hydrogen/air mixture, blockage ratio=0.6; in the second half 10% hydrogen/air mixture, blockage ratio=0.3.
HYCOM-HC20 [34,35]	10% hydrogen-air mixture was filled in a tube of 12.4 m long with of two sections with 2 different diameters: 174 and 520 mm. In the two tubes repeated obstacles with different block ratios were installed. Ignition was made at the end of larger diameter tube, and the propagation of flame was investigated.
Deflagration 1 [34,36]	Combustion experiments have been carried out in obstructed tube. Repeatable obstacles with 2 different blockage ratios at distances equal to diameter were installed. Two typical hydrogen-air mixtures with concentrations of 10% H ₂ (for subsonic deflagration) and 13% H ₂ (for sonic deflagration) have been tested in a tube with different end venting. Ignition at various distances from the open tube.
Kumar 1983 [37]	Large sphere structure vessel (2.3 m diameter) was filled with 29.5% hydrogen-air mixture, ignition was triggered at the center of the vessel and the pressure data was collected through the sensors installed on the wall.
Deflagration 2	Vented hydrogen explosions in a channel on a table without or with 2 baffles from inner wall; ignition centrally at the inner end; concentration variation provided for the empty channel.
Deflagration 3 [38]	A mock-up of a hydrogen refuelling station, which includes a brick wall, two dispensers and simplified steel structure representing a vehicle, was designed. Polythene film is wrapped around the rig, which is then filled with a homogeneous stoichiometric hydrogen-air mixture.
HyIndoor_WP3	Vented 1 m ³ box was filled with 18% hydrogen-air mixture. The ignition was triggered at the center of the wall opposite to the 50cmx50cm vent. Pressures along the vented fire were measured.
Open atmosphere deflagration [39,40]	20m diameter hemisphere balloon was filled with 29.5% hydrogen-air mixture. The ignition was located at the center of the balloon and the pressures were measured.

Table 4: List of DDT experiments in the validation database.

Deflagration to Detonation Transition - DDT	
FZK-R 049809	A 12m long 350mm diameter tube was filled with 15% hydrogen-air mixture. In order to increase the mixing effect, 0.3 block ratio obstacles were installed in the tube. Lighting sensors and pressure sensors were installed in the tube to collect experiment data.
FIKE [41]	Explosion experiments with hydrogen in straight pipes of 3 different diameters (all with length to diameter ratio = 98) were carried out. For the pipe with D=0.1524 and L=15m, 6 different gas concentrations were tested.

Table 5: List of detonations experiments in the validation database.

Detonations	
Hemispherical Det. [42]	Detonation of 29.05% hydrogen-air quiescent mixture in the 53 m ³ hemispherical balloon (diameter 2.93 m). Central point ignition source.
KI_RUT_hyd05 [43]	RUT facility was filled with 20% hydrogen-air mixture. Initiation of the detonation wave was accomplished by the 100g TNT located at the corner of the RUT facility “canyon”. Pressure data was collected by the pressure sensors.
KI_RUT_hyd09 [43]	RUT facility was filled with 25.5% hydrogen-air mixture. Initiation of the detonation wave was accomplished by the 100g TNT located at the end of round tunnel. Pressure data was collected by the pressure sensors.

4.0 BENCHMARKING ACTIVITIES

A number of experiments were selected from the validation database to perform CFD benchmarking activities within the project. The CFD benchmark has several purposes. It will provide an indication of the accuracy and the range of applicability of each modelling approach and it will assess the performance of each model for each kind of phenomena. The benchmarking exercise also offers the opportunity to test the stages of the HyMEP and to suggest values for the statistical performance measures. This final step is important because values of statistical performance measures that correspond to a “good” model have yet to be defined for many of the physics scenarios in the HyMEP. The benchmarking activity is on-going and the results from the first phase have been reported in a project deliverable [44]. In Table 6, the current situation of the benchmarking activities is described with the selected experiments and partners participation. A number of results obtained in some of the selected experiments are shown in the following paragraphs.

Table 6: List of current benchmarking activities

Release and Dispersion	
GAMELAN [15,16]	JRC, NCSR, UU
SBEP_21 [17,18]	HSL, JRC.
Ignition	
PRD (Pressure Relief Device) [31, 32]	UU
Deflagrations	
HyIndoor_WP3	KIT
Open atmosphere deflagration [39,40]	NCSR, UU
Detonations	
KI_RUT_hyd05 [43]	KIT
KI_RUT_hyd09 [43]	KIT

4.1 Release and dispersion

In release and dispersion, two experiments were selected by the partners for the first phase of the benchmarking activities: GAMELAN [16] and SBEP21 [17, 18].

The GAMELAN experimental set up [16] is a parallelepiped enclosure with a square base of 0.93m width and 1.26m height. The vent has a square shape with a total area of 32400 mm² (180 x 180 mm). The vent is located in the middle of the wall and 20 mm below the ceiling. Helium is injected in the enclosure through a 5 mm nozzle. The injection point is located in the middle of the floor at a height of 0.21 m and the release rate is 180 NL/min. For the simulations the ADREA-HF CFD code has been used by NCSR. The turbulence model is the standard k-ε including the buoyancy terms and the good performance of the k-ε model in simulating similar cases was already demonstrated by Giannisi et al. [45]. The good agreement between the predicted helium concentrations and the experimental concentrations over the height of the enclosure at steady state is shown in Figure 2. A statistical analysis of the comparison between CFD results and experimental measurements has been performed, using the following statistical performance indicators: the fractional bias (FB) and the normalized mean square error (NMSE), the geometric mean bias (MG) and geometric mean variance (VG). Given C_o as the observed concentration and C_p as the predicted concentrations, the statistical performance indicators are defined:

$$FB = 2 \frac{\overline{C_o} - \overline{C_p}}{\overline{C_o} + \overline{C_p}} \quad NMSE = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o} \cdot \overline{C_p}}$$

$$MG = \exp \left[\ln \left(\frac{\overline{C_o}}{\overline{C_p}} \right) \right] \quad VG = \exp \left[\ln \left(\frac{\overline{C_o}}{\overline{C_p}} \right)^2 \right]$$

where the over-bar stands for the average value. In Table 7, the value of the statistical performance indicators for the steady state are shown in comparison with the ideal values. With FB absolute values below 0.3 and MG values range between 0.7 and 1.3 the model can be considered as a “good” model in terms of atmospheric dispersion. The small values of the NMSE and the VG indicate a random scatter about a factor of two to three. The negative FB value and the MG value below unity reveals that the model overall over-predicts the helium concentration at steady state.

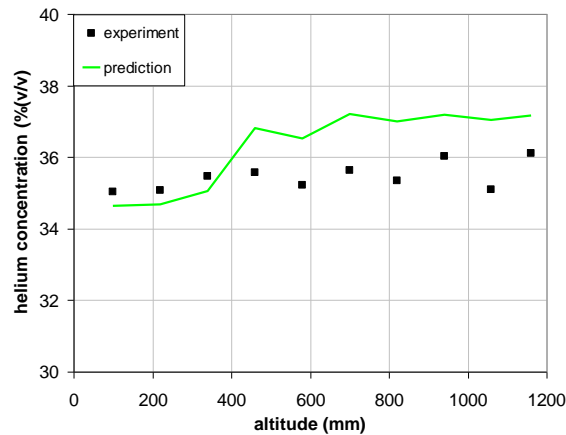


Figure 2. Comparison between the predicted helium concentration and the experimental concentration at steady state (400 s) over the height of the enclosure (GAMELAN facility).

Table 7: Statistical performance indicators for NCSR results on GAMELAN benchmark.

	ideal value	prediction
FB	0	-0.025
NMSE	0	1.52
MG	1	0.97
VG	1	1.001

For the release benchmark SBEP21, simulations of the experiments in the CEA GARAGE facility [17, 18] have been performed by HSL and JRC. The facility is representative of a realistic single vehicle private garage. The experiment was carried out in two phases. In the first phase (the release phase), helium was vertically released with a volumetric rate of 18 L/min for 3740 seconds from a 29.7 mm diameter opening at the centre of the 5.76 m (length) x 2.96 m (width) x 2.42 m (height) facility. After the release stopped, the second phase (the diffusion phase) started and lasted for several thousands of seconds. The commercial code ANSYS CFX has been used in this benchmark. Simulations with the SST (Shear Stress Transport) and laminar model have been performed on an unstructured tetrahedral computational mesh and on a structured hexahedral mesh. The CFD results on the unstructured mesh are in good agreement with the experiment during the release phase but the accuracy of the numerical results decreases significantly during the diffusion phase. On the contrary, with the hexahedral grid the agreement with the experiment remains satisfactory also in the diffusion phase, providing a clear indication that the hexahedral mesh is more suitable than the tetrahedral mesh for the conditions of the selected experiment.

In Figure 3 the comparison between experiment and simulations on a hexahedral mesh for the concentration history is shown for a sensor at 2.37 m height on the left hand side and for a sensor at 0.63 m height on the right hand side. Due to the low flow rate during the release and to the diffusion phase after the release (where flow velocities are certainly smaller than those in the release rate), 2 models for slow flows have been applied: the SST transitional model and the laminar model. The results are in general good agreement for both models.

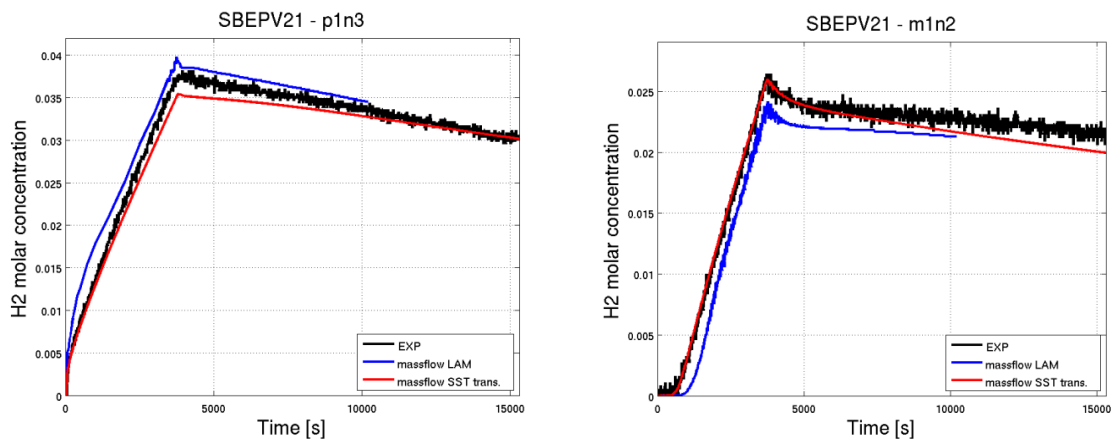


Figure 3. Comparison between experiment and simulations on a hexahedral mesh for the concentration history. Black colour is for the experiment, blue for the simulation with the laminar model and red for the simulation with the SST transitional model. Left hand side: sensor at 2.37 m height. Right hand side: sensor at 0.63 m height.

4.2 Ignition

For the spontaneous ignition benchmark, UU has simulated the experiments that were carried by Golub et al. [31]. In the experiments, the hydrogen was released from a high pressure system into a

channel ending in a T-shaped nozzle mimicking a Pressure Relief Device (PRD). Numerical simulations have been performed for initial hydrogen pressures of 1.5 MPa and 2.9 MPa. The LES model based on the eddy dissipation concept with detailed Arrhenius kinetics for modelling of SGS (Sub-Grid Scale) combustion, and renormalization group theory for modelling of SGS turbulence has been applied. The non-instantaneous burst disk opening plays an important role in the process of ignition due to mixing effect between hydrogen and air. The opening of a membrane has been therefore approximated in simulations by a step-like process with the consecutive opening of 10 concentric sections. For the case with 1.5 MPa initial pressure no auto-ignition has been observed in the simulations and the hydrogen-air mixture temperature has remained well below the combustion temperature. The complete absence of the hydroxyl OH is a confirmation that the combustion chemical reactions are not occurring as illustrated in the right hand side of Figure 4. For the case with initial pressure 2.9 MPa, the ignition occurs at approximately $6.2 \cdot 10^{-5}$ s, after the secondary reflection of the shock wave from the radial channels of the T-shaped PRD as illustrated in Figure 5. The ignition occurs at the location of the leading shock wave secondary reflection. The first reflection occurs when the shock travelling along the axis of the channel reaches the closed end of the PRD. At this time the ignition is not possible as hydrogen is not yet present in that region. Once the hydrogen flows around the edge from the axial into radial channels, it starts mixing with air heated by shocks, providing the necessary conditions for ignition of the mixture. The ignition and its location are confirmed by the sudden appearance of large quantities of hydroxyl OH as depicted on the right hand side of Figure 5. The lack of ignition for the case with 1.5 MPa and the spontaneous ignition at 2.9 MPa are in agreement with the experiment [31].

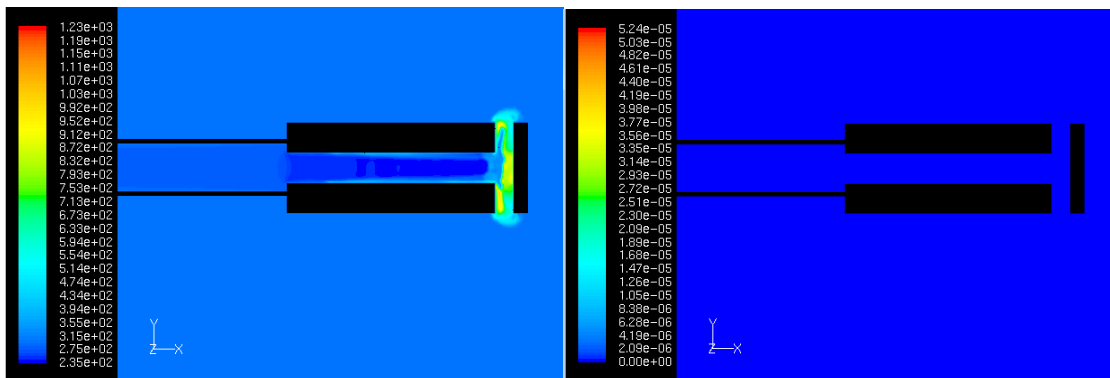


Figure 4. Temperature (left hand side) and OH concentration (right hand side) contours at the axis of the T-shaped PRD at $t=7.46 \cdot 10^{-5}$ s for the case with 1.5 MPa initial pressure.

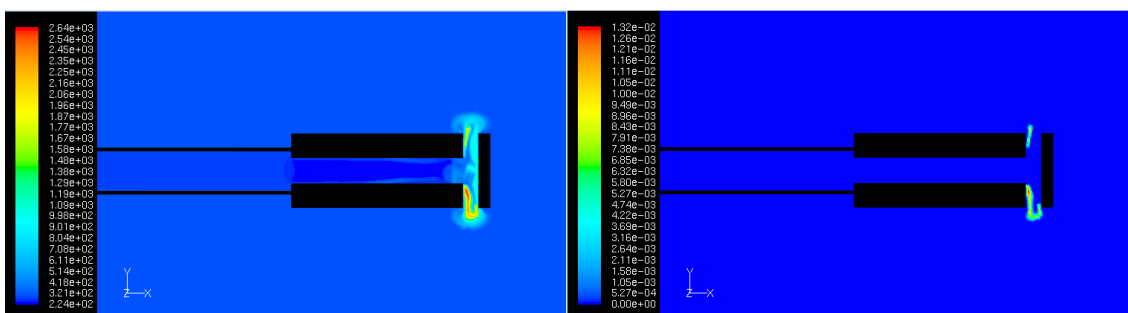


Figure 5. Temperature (left hand side) and OH concentration (right hand side) contours at the axis of the T-shaped PRD at $t=6.65 \cdot 10^{-5}$ s for the case with 2.9 MPa initial pressure.

4.3 Deflagrations

The experiment HyIndoor_WP3 was performed by KIT and it has been reproduced numerically with the code COM3D by KIT. The KIT facility is a chamber similar to a garage where a box with glass walls was placed and filled with a 18% hydrogen-air mixture. The ignition was triggered at the centre of the wall opposite to a 0.5m x 0.5m vent. A photo of the facility is shown in Figure 6. Pressure transducers are located inside and outside the box.

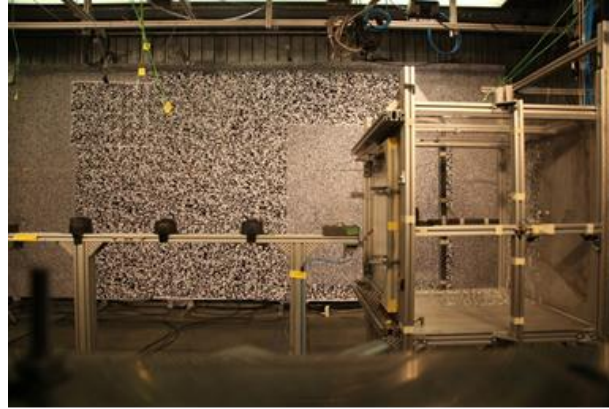


Figure 6. The glass box and transducers inside the KIT facility

The experiment was repeated three times. For the comparisons between the experiment and the simulation, the maximum, minimum and median values of the measurements have been considered. One of the fundamental choices that CFD modellers have to make in the modelling strategy is the level of simplification of the geometrical model. Including all the details of the geometrical configuration is often not feasible because it would require a computational mesh with a very large number of nodes, producing prohibitively expensive computer run-times. Therefore CFD users have to select the main features in the geometry, and neglect some of the elements and details. Since it is difficult to identify the negligible features in the geometry without running simulations, this process usually requires to run a number of calculations. The approach is usually to start with a simplified geometry and add further elements according to the calculation results. In this process, the accessibility to the experimentalists is a crucial aspect because only they know the very small details that are not usually described in the reports of the experiment. Interactions between experimentalists and CFD modellers have been essential also in this case.

Initially the simulations were performed with a very simple model of the geometry as shown in the left hand side of Figure 7. The agreement between the experiments and the simulation is good for the transducers inside the glass box but it is not satisfactory in the sensors outside the box. Therefore a more complex model of the geometry has been generated as shown in the right hand side of Figure 7. Several new elements have been added to the model based on the information that has been provided by the experiment team to the modelling team. The improvements in the simulation results in transducers 8 (outside the glass box) due to the new geometry/model are clear by comparing the 2 graphs in Figure 8. Simulations on even more complex and complete models of the geometry are still on-going.

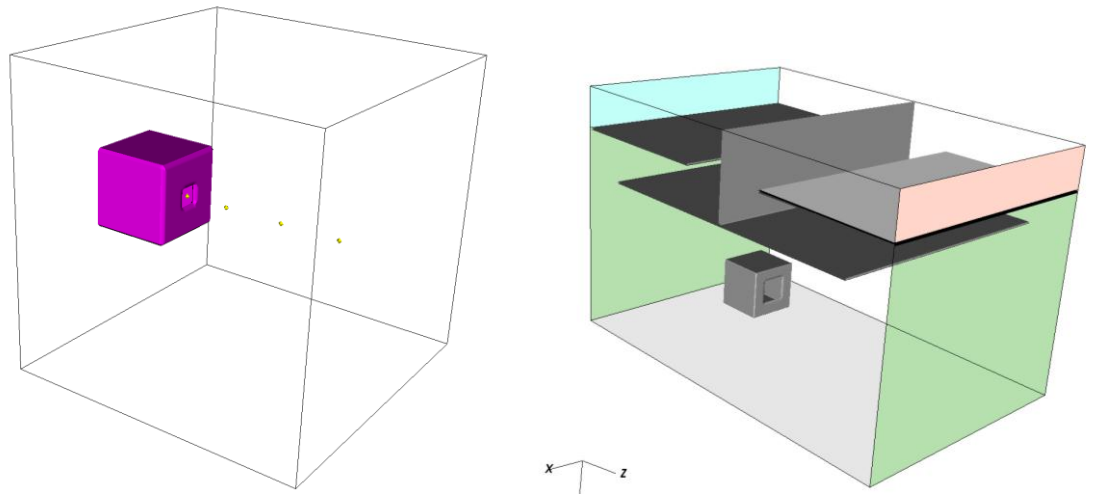


Figure 7. Initial simple model on the left hand side and intermediate complex model of the facility on the right hand side.

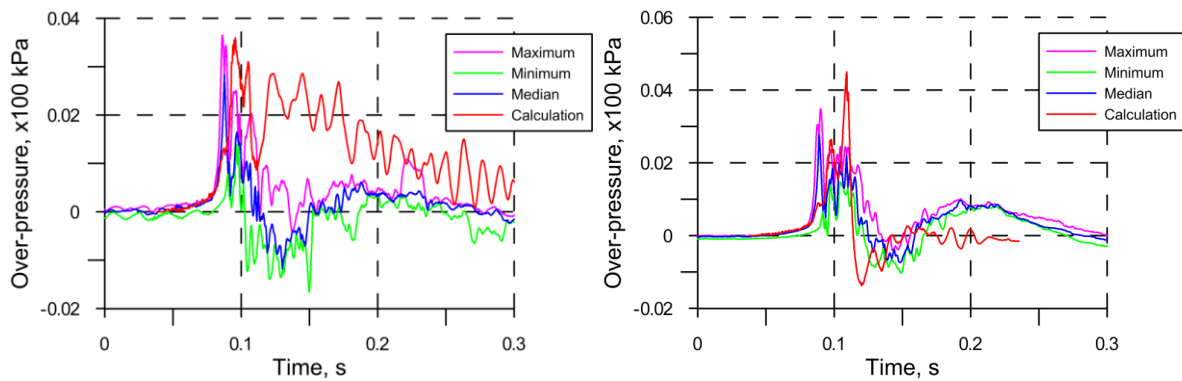


Figure 8. Comparison of the over-pressure history between the experiments and the simulation in transducers 8 (outside the vented box). On the left hand side: results with initial over-simplified geometry/model. On the right hand side: results with the intermediate complex geometry/model.

5.0 CONCLUSIONS

This paper presents some intermediate results from the collaborative SUSANA project whose aim is to develop a Model Evaluation Protocol (HyMEP) for CFD models that are used in safety analyses of hydrogen and fuel cell technologies. The project arose from a recognised need for a framework to support users and developers of CFD software undertaking numerical simulations for the analysis of the safety of FCH systems.

The main stages of the HyMEP are: scientific assessment, verification, validation, sensitivity study, statistical analysis according to the quantitative assessment criteria, and finally the assessment report. A verification database and a validation database are under development in the project and part of the project is a benchmarking exercise which involves the different partners running models against specific scenarios in the validation database.

The experiments that were selected from the validation database for the first phase of CFD benchmarking activities included (but are not limited to):

- Helium release in a vented small box (with a square base of 0.93m width and 1.26m height) through a 5mm nozzle with a 180 NL/min flow rate.
- Helium release in a realistic single vehicle private garage.
- Spontaneous ignition due to the hydrogen release from a high pressure system into a channel ending in a T-shaped nozzle mimicking a Pressure Relief Device (PRD)
- Explosion of a 18% hydrogen-air mixture in a vented 1 m³ box.

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