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Gap Analysis of CFD Modelling of Accidental Hydrogen Release and Combustion

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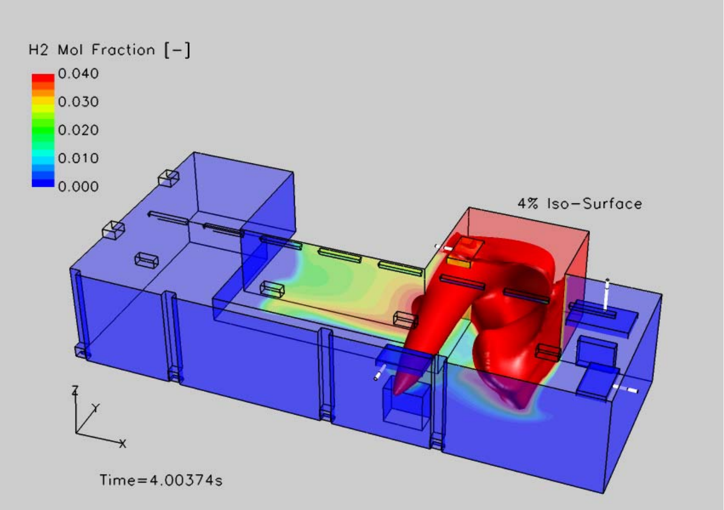

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TABLE OF CONTENTS

EXECUTIVE SUMMARY

Hydrogen is expected to play an important role in the energy mix of a future low-carbon society, as it is stated in the European Strategic Energy Technology Plan of the European Commission (COM 2007 - 723) and in the Hydrogen, Fuel Cells & Infrastructure Technologies Program-Multi-Year Research, Development, and Demonstration Plan of the USA Department of Energy (DoE 2007).

Hydrogen safety issues have to be addressed in order to demonstrate that the wide spread deployment and use of hydrogen and fuel cell technologies can occur with the same or lower level of hazards and associated risk compared to the conventional fossil fuel technologies. Computational Fluid Dynamics (CFD) is considered one of the tools to investigate safety issues related to the production, storage, delivery and use of hydrogen. CFD techniques can provide a wealthy amount of information on the dynamics of hypothetical hydrogen accident and its consequences. The CFD-based consequence analysis is then used in risk assessments. In this context a workshop was organised at the Institute for Energy (JRC) in Petten, Netherlands with the purpose of identifying the gaps and issues in CFD modelling of hydrogen release and combustion. The report describes the main findings of the workshop.

A hydrogen accident occurs usually following a typical sequence of events: an unintended release, the mixing of hydrogen with air to form a flammable mixture, the ignition of the flammable cloud and depending on the conditions, a fire or an explosion (deflagration or/and detonation). For each stages of the accident, the critical CFD issues have been identified and prioritised.

Beyond the specific issues of CFD modelling that are described for each accident stage in the report, some general modelling issues can be found in all stages:

- lack of an extensive validation of CFD codes/models that covers all the relevant range of conditions that can be found in hypothetical accident scenarios e.g. in terms of geometrical lay-out, leak flow rates, etc.
- lack of a CFD validation protocol for hydrogen like it exists for Liquefied Natural Gas (LNG): the Model Evaluation Protocols (MEP) for assessment of models for accident consequences, with guidance on evaluating models in terms of scientific assessment, verification and validation.
- lack of a database of experiments for validation of hydrogen models.
- in some cases, lack of complete and accurate experimental data for the CFD validation.

1. INTRODUCTION

A workshop was held at the Institute for Energy/JRC (Petten, The Netherlands) in order to identify the gaps in CFD modelling and simulation of hydrogen release and combustion. The report describes the findings and the results of the workshop.

Computational Fluid Dynamics (CFD) methods are increasingly used for hydrogen safety analysis since they can provide relevant information for the hazards and risk assessment of hydrogen technologies such as pressure and thermal loads, e.g. the overpressures generated by an explosion or the length of a jet fire. CFD simulations can provide a valuable contribution to the engineering design of safer hydrogen infrastructure and development of innovative mitigation measures and procedures.

Numerical techniques, as well as analytical and experimental methods have been developed and used to investigate open issues in fluid dynamics. Those three approaches are strongly interlinked and constitute the main research tools in modern science. The governing equations of the motion of non-reacting and reacting fluids are the Navier-Stokes (NS) equations that can not be solved analytically. Therefore it is necessary to use numerical techniques together with validation experiments to close the knowledge gaps related to the flow behaviour such as in the case of accidents with liquefied or gaseous hydrogen.

In order to apply CFD techniques to real-scale problems, one has to be confident about the level of reliability and accuracy of the numerical tools. To achieve the required level of confidence, the CFD codes/models must undergo an assessment procedure according to the steps depicted in Figure 1.

Verification is defined as the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model (Oberkampf et al., 2008). Verification must assure that the set of partial differential or integral-differential equations are solved correctly. Verification does not address the issue of whether the mathematical model represents correctly the real world, e.g., physics. Verification is performed by the code developers and in this report it is reasonable to assume that all the numerical codes have been well verified.

Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Validation shows how accurately the computational model simulates the real world (Oberkampf et al., 2008) or rather specific conditions of a test or an experiment that are designed to represent the "real world".

In some cases no validation calculations have been carried out for a specific problem because the experimental data are too few or non-existent. In those cases, only demonstration simulations can be performed since it is possible only to demonstrate that the CFD code potentially has the capability of simulating the problem, at least from the qualitative point of view (Smith, 2009).

In hydrogen accident scenarios, the physical phenomena occur following a typical sequence of events: release, dispersion, ignition, fire or explosion. The initial phase in a hydrogen accident is the accidental release from a tank or a hydrogen system, followed by the dispersion phase during which hydrogen mixes with air. At that stage auto-ignition or accidental ignition of the flammable mixture may occur. Depending on the local conditions at the time of ignition, the combustion process can develop into a fire or into an explosion (a deflagration or a detonation). The structure of this report follows the typical sequence of the events during a hydrogen accident scenario aiming at identifying the gaps in the following main topics: release and dispersion, ignition/auto-ignition, fires, deflagrations, detonations (including deflagration to detonation transition or DDT), and accident consequences. At the end of each paragraph, a list of the identified gaps for each topic can be found. The gaps have been prioritised as more urgent/critical or medium urgent/critical or less urgent/critical issues.

The previous works of Bengaouer et al. (2007), Jordan (2009), Kotchourko (2009), Molkov (2009) and Tchouvelev (2008) about hydrogen safety gaps have been taken into account in the analysis.

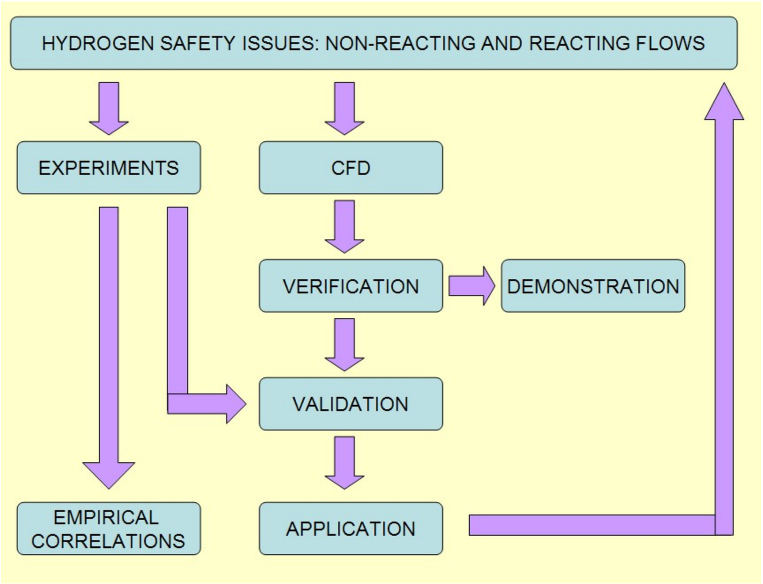

Figure 1: Diagram for CFD application and validation procedure.

2. GENERAL ISSUES

In this paragraph, some of the modelling issues that are common to several stages of the accident scenarios are described.

Gaps can be identified at different levels: lack of fundamental knowledge or understanding of some aspects of the physical phenomenon resulting in inadequacies and deficiencies of the models; lack of experiments for validation; inability of the CFD model to reproduce and predict the phenomenon from the qualitative and/or quantitative point of view.

Turbulence is still one of the major open issues in modern physics, although many progresses have been performed in the last decades. In CFD three main approaches are currently applied to address the turbulence issue. In Direct Numerical Simulations (DNS), the whole range of turbulent scales is captured directly in the extremely fine computational mesh and therefore no model for turbulence is required. Since DNS is computationally very expensive, this approach is restricted to flows with low Reynolds number and extremely small computational domain. Nevertheless DNS is a powerful tool of investigation, improving the fundamental understanding of turbulent flows and providing essential information for developing turbulence models, especially sub-grid scale (SGS) models for Large Eddy Simulations (LES). In Figure 2, it is shown an example of DNS simulations where the effect of the Lewis number on the flame is investigated (Chakraborty and Cant, 2005).

In Large Eddy Simulations (LES), the largest turbulent scales are captured by means of the mesh while the effects of the smaller scales are modelled using SGS closure models. In Very Large Eddy Simulations (VLES), the filter and the computational grid are too coarse to resolve 80% of the turbulent kinetic energy (Pope, 2000). In Reynolds Averaged Navier-Stokes (RANS) equations, the averaged fluid governing equations of the fluids are solved, providing the mean values of all quantities. One of the major drawbacks of this approach is that it requires models for turbulence closure. Traditionally RANS techniques have been the most applied method for industrial applications because they are the most convenient from the computationally point of view. Two known issues with RANS turbulence models are the reliability of the models in complex flow environments, in particular in presence of turbulent mixing and in regions of flow separation, and the predictions of laminar-turbulent transition (Hirsch et al., 2009).

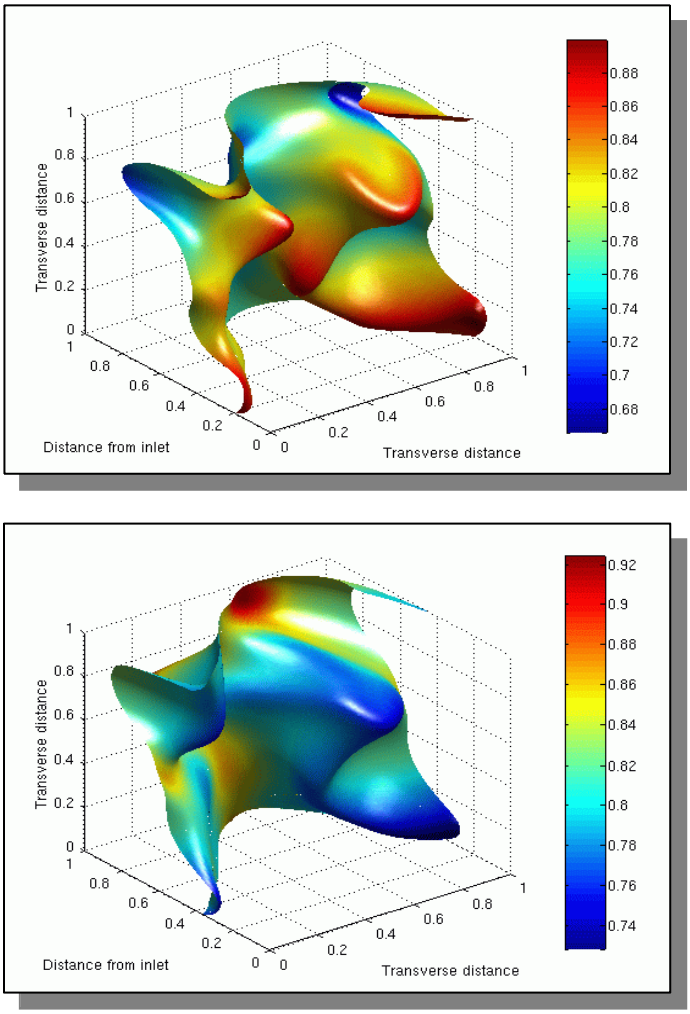

Figure 2: Instantaneous pictures of the progress variable iso-surface (c=0.8) coloured by local non-dimensional temperature. Lewis number is equal to 0.8 (top) and to 1.2 (bottom) (Chakraborty and Cant, 2005).

Another important issue is related to the mesh resolution. Some combustion phenomena such as spontaneous ignition or Deflagration to Detonation Transition (DDT) require an extremely fine mesh resolution of the order of microns that is not affordable in simulations in real-scale configurations. In those cases CFD is capable of describing certain phenomena only in small domains and not in large scale industrial applications due to the current limitations of the computer resources. In the last case those phenomena can only be modelled on a SGS level. Since computer power has been increasing constantly in the last decades, it is easily foreseeable that CFD applications will continue to benefit from the constantly increasing computer power.

An important distinction in CFD modelling is the difference between the CFD capability of reproducing the experimental data and the capability of predicting the experimental measurements. Within the CFD community benchmarking activities are frequently performed. Simulation results are compared to experimental data that are known to the modellers before the beginning of the validation exercise. In this case, simulations show the capabilities of CFD codes/models of reproducing the experiment. Less frequent are the blind simulation tests where the experimental data are not known to the CFD experts before the calculations and they are revealed only after the calculations. Blind tests in many cases demonstrate the current predictive capability of a CFD tool. One open question is whether simplified models/codes calibrated on numerous experiments may have higher "predictive" capabilities compared to more sophisticated physical models which are "validated" against lesser amount of experiments. The CFD benchmarking activities have to be shifted from a simple comparison of CFD tools in reproducing one particular experiment to a comparison of underlying physical models, including their advantages and deficiencies, and their capability to reproduce a range of experiments without changing the model parameters.

For other CFD applications, Model Evaluation Protocols (MEP) for assessment of models for accident consequences has been developed. For example, Health and Safety Laboratory (HSL, UK) on behalf of National Fire Protection Association (NFPA, USA) developed a MEP for Liquefied Natural Gas (LNG) dispersion with guidance on evaluating models in terms of scientific assessment, verification and validation (Ivings et al., 2007, 2008). The report provides a uniform and structured approach to reviewing all existing and newly developed models. Moreover, a database of experiments for validation of LNG models was established as described by Coldrick et al. (2009). Guidelines for CFD applications for LNG safety analysis (such as for a computational domain, a grid, boundary and initial conditions) are provided by Luketa et al. (2007). However, for CFD applications related to hydrogen safety issues the situation is different. Within the European Network of Excellence HySafe (www.hysafe.net), some interesting validation work has been performed by means of several Standard Benchmark Exercise Problems (Gallego et al., 2007) (Garcia et al., 2010) (Baraldi et al., 2009, 2010) (Jordan et al., 2007) (Makarov et al., 2009, 2010) (Papanikolaou et al., 2010) (Venetsanos et al., 2009, 2010), applying the MEGGE (1996) evaluation protocol originally developed for hydrocarbon explosions. Nevertheless no specific model evaluation protocol, no validation database and no specific CFD guidelines have been developed and universally accepted for hydrogen applications.

3. RELEASE AND DISPERSION

During the hydrogen release into the atmosphere, a hydrogen-air cloud will be generated and part of it could be flammable. The conditions in the hydrogen-air cloud at the ignition time such as the amount and the distribution of hydrogen concentration within the flammable cloud, the flow field and the level of turbulence within the cloud, the level of spatial congestion and confinement are all relevant parameters that can significantly affect the strength of the explosion. Therefore it is essential that the computational models are capable of correctly describing this phase of the accident in order to capture the following phase with a sufficient level of accuracy.

PERMEATION

Permeation is the molecular diffusion of hydrogen through the walls of a container vessel, piping or interface materials (SAE, 2009). Because of this phenomenon, hydrogen is released continuously at extremely low rate from the storage system. This phenomenon is an issue for tanks with non-metallic liners (Type 4 tanks) while it is considered negligible for metallic tanks and for tanks with a metallic liner (Types 1, 2 and 3). Proposals for vehicle regulations and standards for hydrogen systems provide thresholds on the allowable rate of hydrogen permeation from Type 4 tanks (Adams et al., 2009). Permeation issues were recently addressed within the InsHyde internal project of HySafe Network of Excellence, co-funded by the European Commission (Adams et al., 2009a, 2009b) (Venetsanos et al., 2009a) (Saffers et al., 2009) (Cariteau et al., 2009) in order to investigate the existing rates proposed in the draft ECE compressed gaseous hydrogen regulation and the various versions of ISO/DIS15869 (Gaseous Hydrogen and Hydrogen Blends - Land Vehicle Fuel Tanks). The focus of the work was to provide an allowable permeation rate for the draft EC regulation for type-approval of hydrogen powered motor vehicles and the container requirements in the UN ECE WP29 GTR proposal. The work included experiments with small mass flow rate releases of helium and CFD simulations. The dispersion experiments were performed by Cariteau et al. (2009) in the CEA (Commissariat à l'Énergie Atomique) Garage facility (5.76m x 2.96m x 2.4m), using helium (for safety reasons) released vertically from a 7 cm diameter hole in the centre of the floor. CFD validation was performed by Venetsanos et al. (2009a, 2009b) using the ADREA-HF code. Figure 3 shows a comparison between measured and predicted helium concentration for a period of approximately 2.3 days. Agreement between CFD, homogeneous model and experimental data is quite satisfactory.

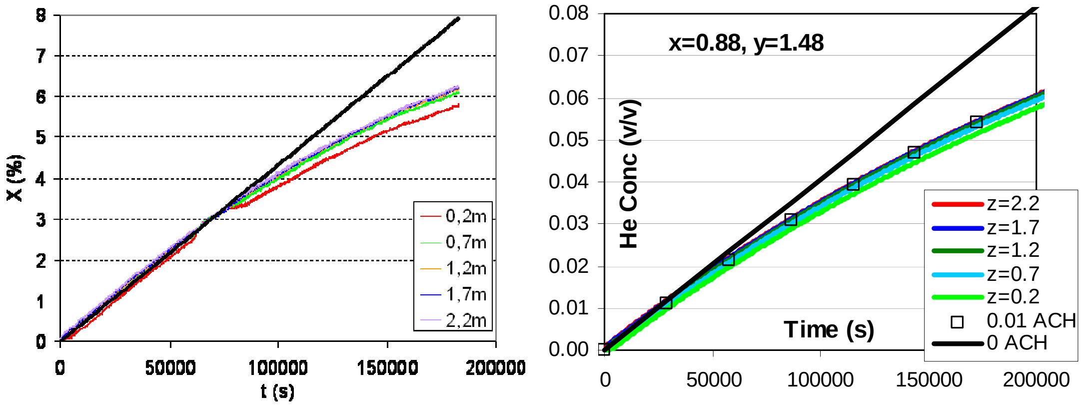

Figure 3: Comparison between measured (left-hand side) and predicted (right-hand side) concentration time series for a period of approximately 2.3 days (bottom). Open boxes and black line show the homogeneous model solutions

The dynamics of dispersion of permeated hydrogen from a storage tank (L=0.672 m, D=0.505 m, hemisphere at each end with D=0.505 m, V=0.2 m^3, surface 1.87 m^2) with floor clearance of 0.5 m in a centre of typical garage of $L\times W\times H$=5×3×2.2 m (V=33 m^3) with still air at temperature T= 298 K performed at the University of Ulster are shown in Figure 4. A volumetric release of hydrogen in a thin layer around the tank surface was assumed in the simulation. Preliminary numerical simulations showed that there is no 100% hydrogen concentration at the tank surface during the permeation. For this reason the authors decided to model the source of permeated hydrogen using volumetric source of hydrogen in a thin layer (1 mm thickness control volumes) around the tank surface. In this particular case the permeation rate was J=1.40×10^{-6} mol/s/m^2 (1.14 NmL/hr/L of tank volume): equivalent mass source term in CFD S_{H2}=2.61×10^{-8} kg/m^3/s. Time to reach lower flammability limit (LFL) of 4% in fully sealed garage with chosen storage tank and permeation rate will be 240 days (assumption of uniform dispersion). The characteristic time for hydrogen diffusion through the height of the garage is $Height^2/D_{H2}$ (at 298 K the diffusion coefficient is D_{H2}=$7.79.10^{-5}$ m^2/s) and is much shorter, $2.2^2/7.79.10^{-5}$=62051 s or 0.7 days. This implies that we could expect quasi-uniform distribution of hydrogen in a garage without ventilation during dispersion of permeated hydrogen. Indeed, numerical simulations confirmed that in-homogeneity of hydrogen distribution is negligible (difference between hydrogen concentration at the ceiling and on the bottom is about 0.003% by volume, which is far below the lower flammability limit of 4% by volume). It is expected that tests with high pressure hydrogen of Type 4 in sealed enclosure will confirm this finding.

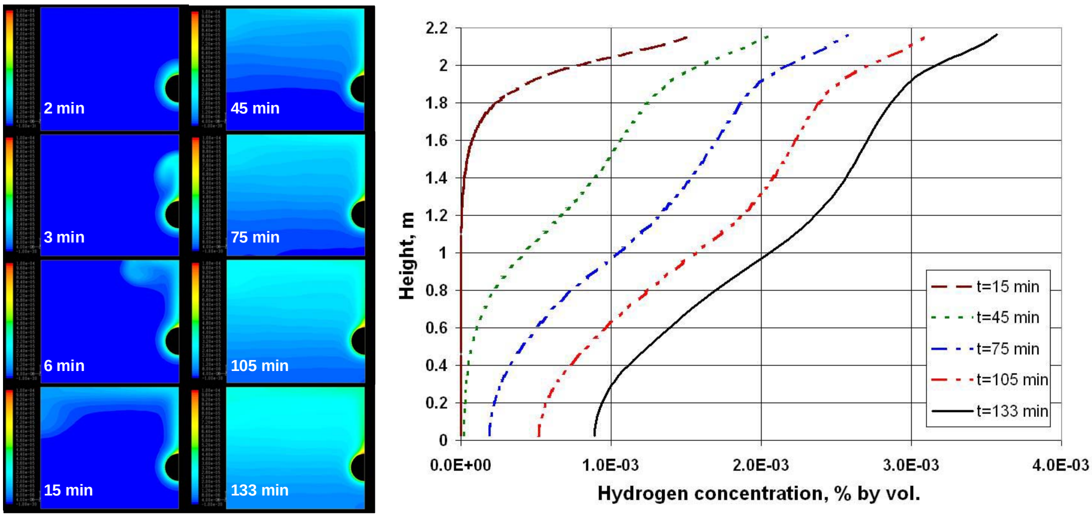

Figure 4: 2D-slice distribution of hydrogen in a half of the typical garage (left-hand side) and distribution of hydrogen by height at location between wall and the tank (right-hand side) with time

In permeation no very critical/urgent issues have been identified. Nevertheless some issues are still open:

- Experiments with dispersion of hydrogen permeated from real tank in room-like enclosure with controlled ACH (air change per hour) or sealed are required.
- More experiments are required for validation, extending the existing CEA database, such as experiments with the very limiting low flow rates used (0.03 L/min).
- Experiments/simulations using the real release geometry to investigate the effect of geometry (i.e. the storage cylinders instead of a nozzle).
- Experiments/simulations including the car/bus geometry to investigate the effects on the dispersion pattern and the conditions of dangerous hydrogen accumulation within the vehicle compartments (such as luggage compartment, passenger compartment).
- Effect of natural ventilation parameters (ACH; size, location and number of vents; wind, etc) on distribution of permeated hydrogen within enclosure are not clarified yet.
- CFD validation using different turbulence models/codes available to stakeholders.

GASEOUS HYDROGEN

Compared to liquid hydrogen, a larger number of experimental work and numerical simulations have been carried out with gaseous hydrogen.

Since helium is not flammable and is the gas with the most similar features and behaviour to hydrogen regarding the dispersion properties, helium is often used as a substitute for hydrogen in experimental studies of release. A list of experimental investigations on helium and hydrogen release is provided in *Table 1*.

Depending on the system pressure, the flow through the leakage can be subsonic or sonic. Jets could be buoyancy or momentum dominated.

Releases from high pressure systems are characterised by under-expanded jet, which undergoes one or a series of normal and oblique shocks, depending on the pressure at the nozzle, with the first shock being a normal shock often referred to as the Mach disk. Different approaches are being used to model the under-expanded jets in the region close to the release source.

Capturing and completely describing the complex shock structure at the leakage requires a very fine computational mesh in a near to nozzle field and, unfortunately, unfeasible computer run-times if dispersion in a far field has to be simulated on the same grid.

Example of LES of under-expanded supersonic jet in a near field performed at the University of Ulster is shown in Figure 5 indicating high Mach numbers of flow within the barrel shock and highly non-uniform distribution of flow velocity after the Mach disk.

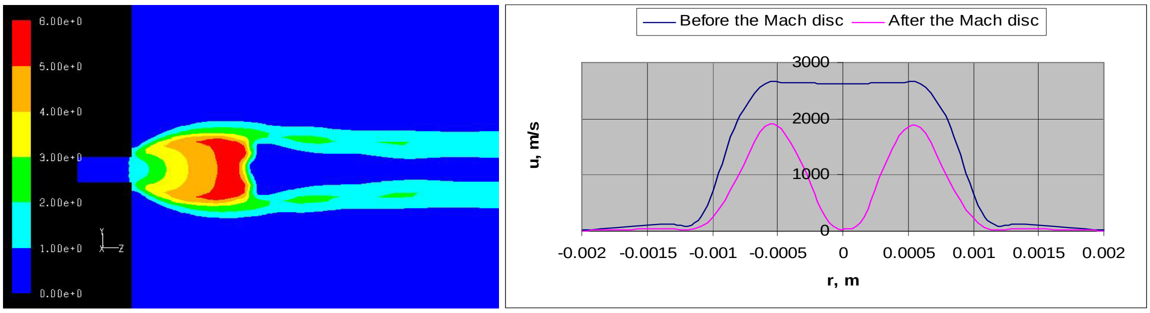

Figure 5: Under-expanded jet of hydrogen to air: flow Mach number (left-hand side); flow velocity before and after the Mach disk (right-hand side).

Table 1: Experiments of hydrogen and helium releases.

Hydrogen Experiments	**Helium Experiments**
Cerchiara et al., (2009)	Aihara et al., (1974)
Desilets et al., (2009)	Cariteau et al., (2009a, 2009b)
Friedrich et al., (2007, 2009)	Caron-Charles et al., (2001)
Fürst et al., (2005)	Chan et al., (1997)
FZK report, (2005)	Cheng et al., (2005a)
GEOMET final report IE-2647,	Djilali et al., (2009)
Hayashi et al., (2004)	Gupta et al., (2007)
Houf and Schefer, (2008)	Keagy and Weller, (1949)
Lacome et al., (2007)	Korobtsev et al., (2009)
Mattei et al., (2009)	Paillere and Tkatschenko, (2004)
Merilo et al., (2009)	Panchapakesan and Lumley, (1993)
Royle and Willoughby, (2009)	Pitts et al., (1986, 2009)
Schefer et al., (2008)	Swain et al., (1999)
Seifert and Giesbrecht, (1986)	Way Libby, (1970)
Shebeko et al., (1988)	
Shirvill et al., (2005, 2006)	
Swain et al., (1998, 2004)	
Takeno et al., (2005)	
Tanaka et al, (2005)	
Xiao et al., (2009)	
Chaineaux et al., (1991)	
Ruffin et al., (1996)	
Okabayashi et al., (2005)	

There are currently a number of investigations aiming at identifying the level of details that are necessary to be captured in the shock structure in order to correctly describe the dispersion of hydrogen in a far field.

Only a few numerical studies are concerned with highly under-expanded H_2 jets into the atmosphere because the very low density and the high sonic speed of H_2 render the numerical simulation strongly nonlinear and extremely challenging (Xu et al. 2005). Xu et al. (2005) suggested a two step approach to overcome the very demanding requirements for the mesh resolution in the sonic release region. They performed the numerical simulation of the sonic release region close to the source, using a very fine mesh resolution in a small computational domain representing only the small region where the complex shock structure is formed. Subsequently they used the information on the flow from the first simulation as input for a second simulation with a much larger computational domain and with a coarser mesh resolution, representing the complete real scale configuration without the near-source region. The authors (Xu et al. 2005) mentioned the lack of suitable experimental data for quantitative comparison to validate their numerical work, especially in the near release area.

A common simplified approach based on the concept of notional nozzle or pseudo source or effective diameter (Birch, 1984, 1987), (Ewan and Moodie, 1986), (Houf and Schefer, 2007) is followed to overcome the numerical difficulties of modelling the actual source. In this approach the region with the complex shock structure is not included in the simulations and the release is assumed to start from a region downstream of the Mach disk. The diameter and flow velocity at the pseudo source are calculated by applying mass and momentum conservation between the leakage and a point beyond the Mach disk where the pressure of the jet is equal to the ambient pressure. The pseudo-source approaches may incur in some inaccuracies due to the introduced assumptions (neglect of air entrainment into the jet, uncertainty of the assumed temperature) (Xu et al., 2005). In the HySafe Biennal Report on Hydrogen Safety (2007) it is suggested that such kind of approaches should be further investigated and validated in all relevant conditions.

In the work by Tchouvelev (Tchouvelev, 2008) a comparison between the actual and the pseudo-source approach of a H_2 release from a 430 bars system was made. It was found that the pseudo-source approach produced 25-30% longer extents in the flammable cloud than the actual leak modelling. The author stated that the main reason for this difference is the use of real gas hydrogen properties in the actual leak approach while the notional nozzle approach uses the ideal gas law. Another contributing factor is the different input velocity of sound used in the two approaches. In the actual leak approach, the velocity of sound is calculated at the critical temperature (1189 m/s) whereas in the pseudo-source approach at ambient conditions (1305 m/s).

Recently an alternative approach to calculate notional nozzle diameter, based on the conservation of mass and energy and the use of Abel-Noble equation to account for non-ideal behaviour of hydrogen at high pressures, has been suggested (Molkov, Makarov, Bragin, 2009). Validation of this approach coupled with the use of the similarity law by Chen and Rodi against available experimental data on axial decay of hydrogen from underexpanded jets (Chaineaux et al., 1991: storage pressure 100 bar, orifice diameter 5, 12, 24 mm; Ruffin et al., 1996: 40 bar, 25-100 mm; Shirvill et al., 2005-2006: 10-172 bar, 1-12 mm; Okabayashi et al., 2005: 400 bar, 0.25-2 mm; Kuznetsov et al., 2005: 53-161 bar, 0.16-1 mm) is shown in Figure 6.

In the last version of the Phenomena Identification and Ranking Table (PIRT) report by Bengaouer et al., (2007) the modelling of the mixing process for chocked flow releases was identified as a phenomenon for which still some uncertainties remain although it is understood on the whole.

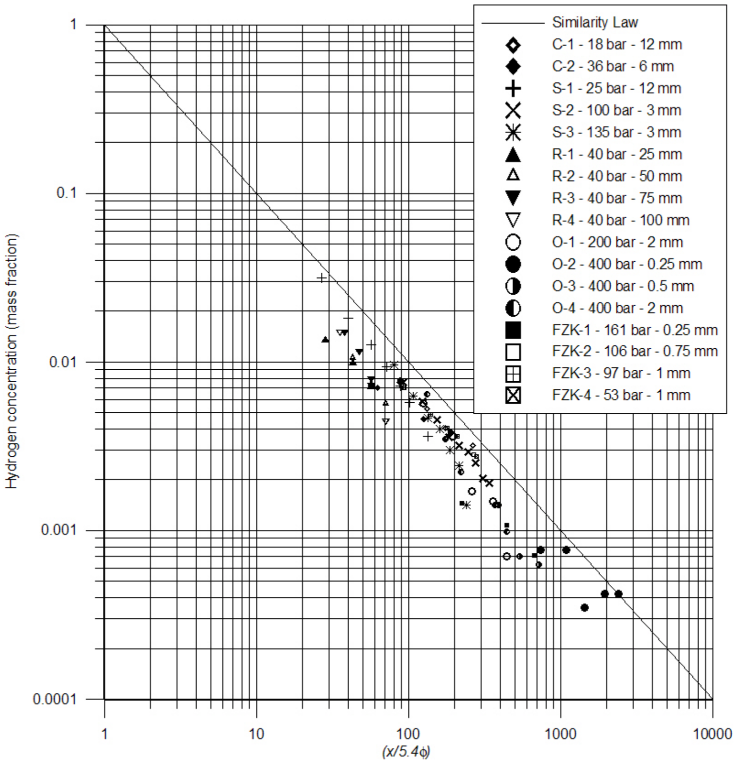

Figure 6: Validation of the under-expanded jet theory (Molkov, Makarov, Bragin, 2009) by experimental data on hydrogen concentration decay along the jet axis.

Recently it was found that the presence of a surface in the proximity to the jet centreline result in an increase in the length of the flammable cloud compared to a free jet (Hourri et al., 2009; (Benard et al., 2009). Since the pipes and components are normally located in proximity of surfaces such as the ground/floor or walls, this effect should be thoroughly investigated.

The deviation of hydrogen behaviour from the ideal gas law grows with increasing pressure as shown by Mohamead et al. (2005) and Cheng et al. (2005b). Therefore at high pressure real gas laws have to be applied and real gas properties is another relevant area of investigation.

Based on the above, it is important to assess in a more systematic way the effect of using different source modelling approaches on the downstream behaviour of the jet.

Recently it has been demonstrated by a phenomenological theory of under-expanded jets, developed at the University of Ulster, and by LES that pressure losses in piping system have essential effect on mass flow rate and hence dispersion of hydrogen in a far field, in particular on the size of flammable envelope (Molkov and Bragin, 2009).

Many numerical investigations on hydrogen (or helium) release and dispersion have been performed: Angers et al. (2005), Babic et al. (2008), Barley et al. (2007, 2009), Cheng et al. (2005a, 2005b), Gallego et al. (2007), Heitsch et al. (2007), Jordan et al. (2007), Khaksarfard et al. (2009), Matsuura et al. (2008, 2009a, 2009b), Middha et al. (2009a, 2009b), Mukai et al. (2005), Nilsen et al. (2007), Papanikolaou et al. (2005, 2007, 2009a, 2009b, 2009c), Peneau et al. (2009), Sommersel et al. (2009), Tchouvelev et al. (2007a, 2007b), Venetsanos et al. (2009a, 2009b, 2008, 2003), Vudumu et al. (2009), Xu et al. (2005), Zhang et al. (2007), Zheng et al. (2009), Molkov et al. (2009).

A relevant number of issues are still open in gaseous hydrogen dispersion.

Very urgent/critical issues

- CFD simulation/validation of releases in real-complex configurations such as with barriers, obstacles, confinement, jet impingement, etc.
- Dispersion of hydrogen releases in enclosures with natural or forced ventilation (effect of mass flow rate and direction; location, number, shape and area of vents; wind, etc.).
- Validation of notional nozzle theories, especially with small diameter of the nozzle below 1 mm when effect of pressure losses is significant.
- Effect of the wind on outdoor releases in areas with complex surroundings such as in urban streets.
- Surface effects on jet release depending on release pressure, release orifice and proximity to surface (both horizontal and vertical).
- Structure and hydrogen concentration decay in plane jets (from cracks).
- Interaction of multiple jets.
- Accounting for non-ideal behaviour of hydrogen at high pressures in CFD codes

Medium urgent/critical issues

- Effect of turbulence modelling, inter-comparison of RANS and VLES, hybrid models.
- Transient effects in high momentum jets.
- Dynamics of transition from momentum- to buoyancy-controlled flows in under-expanded hydrogen releases.

Less urgent/critical issues

- Minimum mesh resolution that is required for RANS and VLES in real scale configurations to describe the actual release source in the approach without the notional nozzle modelling.

- Downward free and impinging jets: effect on the flammable envelope as compared to vertical jets.

- Buoyancy effects on Gaussian distribution in the jet.

- Dynamics of unsteady releases (blow-downs, hydrogen bubbles, hydrogen puff, etc.).

- Cold jets in humid air (momentum sink or dead jets due to vapour condensation and super-entrainment into the jets).

LIQUID HYDROGEN (LH2)

Release and dispersion of liquid hydrogen is an area where there is a significant lack of both experimental and modelling work. Very few experiments of LH_2 spillages are available in the scientific literature (Witcofski and Chirivella, 1984), (Chirivella and Witcofski, 1986), (Dienhart, 1995), (Verfondern and Dienhart, 1997). Also, for liquid release as it happens for gas release, helium is sometimes used as replacement for hydrogen such as in the experiments of liquid helium spillages by Proust and co-workers (Proust et al., 2007). Given the low number of liquid hydrogen experiments, a few validation studies can be found in the literature (Molkov et al., 2005), (Venetsanos et al., 2007) (Verfondern and Dienhart, 2005), (Middha et al., 2009), (Winters and Houf, 2009).

Some fundamental knowledge gaps exist for LH_2 release.

<u>Very urgent/critical issues</u>

- The physical properties of liquid hydrogen (properties of H_2 - but also of O_2 N_2, H_2O - close to saturation, departure from the ideal gas law at low temperature).

- Effect of humidity and temperature on release.

- Effect of buoyancy and wind on release.

- Two – phase jets

Medium urgent/critical issues

- Conductive, convective and radiative heat transfer issues between the cold hydrogen and the surrounding environment including air and the ground.
- Phase change issues such as the hydrogen evaporation and the condensation of nitrogen, oxygen, and water in the air.

The lack of experiments that can close the above open issues is a major obstacle to the validation of CFD tools and their applications. In addition, heat transfer and turbulence modelling at low temperatures is a challenging task.

4. IGNITION AND AUTO-IGNITION

A review of the postulated mechanisms for spontaneous ignition of hydrogen leaks can be found in the paper by Astbury and Hawksworth (2007): the reverse Joule–Thomson effect, the electro-static ignition, diffusion ignition (ignition behind a shock wave), sudden adiabatic compression and hot surface ignition.

In many CFD calculations of premixed flame propagation the ignition is modelled in a simple fashion, e.g. by artificial raising the temperature and the combustion products concentration in a limited number of computational cells or one cell in the ignition position. The simplified ignition model seems to perform well enough in the majority of the combustion cases if the purpose of the investigation is to study the flame propagation and the associated overpressures and heat fluxes after the ignition.

If the emphasis of the CFD investigation is to understand and predict if and when the spontaneous ignition occurs, a more sophisticated modelling is required. It is well known that hydrogen does not necessarily ignite spontaneously when released at high pressures (Astbury and Hawksworth, 2007) and identifying the conditions under which the self-ignition occurs is a major task for current investigations.

Dryer et al. (2007) stated that more experimental and computational work is required to quantitatively determine the envelope of parameters combinations that mitigate or enhance spontaneous ignition characteristics of compressed hydrogen as a result of sudden release from a high pressure system. Some of the relevant parameters are the hydrogen pressure inside the vessel, the temperature of the compressed hydrogen and the surrounding air, and the length and the diameter of the pipe/opening through which the gas is released.

When high-pressure hydrogen is suddenly discharged into air, a shock wave is formed and it compresses/heats the air, which mixes with hydrogen at the contact surface. This causes a temperature rise of the hydrogen–air mixture, with the possibility of spontaneous ignition. If the ignition occurs inside the pipe, when the flame reaches the pipe exit, it can develop in a sustained jet fire or it can be quenched during the strong expansion that it undergoes when it comes out of the pipe. This phenomenon has been investigated in several experimental and numerical studies.

Experimental work on the topic was carried out by Dryer et al. (2007), Golub et al. (2007, 2008, 2009a, 2009b), Mogi et al. (2008, 2009), Desilet et al. (2009). Reported at FLUCOM 2009 conference last results of the Golub's group show that spontaneous ignition is possible for as low storage pressure as 13.5 bar.

Numerical investigations were performed by Bauwens et al. (2009), Bragin and Molkov (2009a, 2009b), Golub et al. (2007, 2008, 2009a, 2009b), Lee et al. (2009), Radulescu et al. (2007), Wen et al. (2009), Xu et al. (2008, 2009a, 2009b), and Yamada et al. (2009a, 2009b). Imamura et al. (2009) investigated ignition at ventilation duct outlet by electrostatic discharge.

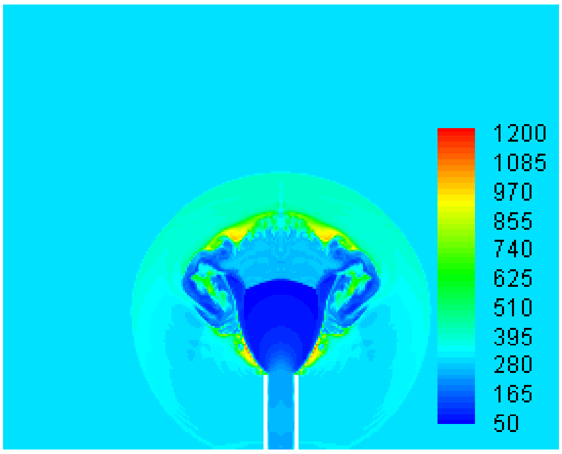

Figure 7: Temperature field generated by the hydrogen release from a high pressure tank (100 bars) through a pipe (courtesy of Prof. Wen and co-workers; Kingston University).

From the qualitatively point of view, it has been shown that CFD is capable of reproducing the ignition inside the pipe (Wen et al., 2009), (Bragin and Molkov, 2009a, 2009b) and the experimentally observed phenomenon of flame separation in the atmosphere (Bragin and Molkov, 2009a, 2009b). From the quantitative point of view, extensive validation work is still required.

The transition from the ignition to self sustained jet fires is more challenging and so far there are very few simulations of that phenomenon and only at small scales (Bragin and Molkov, 2009a, 2009b). Describing the transition requires very fine mesh resolution that can not be directly applied in three-dimensional real-scale situations.

Another area of uncertainty that requires validation is the modelling of the transient during the opening/rupture of the membrane or valve that separates the high pressure hydrogen from the ambient pressure air.

An extremely relevant open issue concerns the application of CFD to hydrogen explosions for hazard and risk assessment and the role of the ignition location. Given an accident scenario, release simulations provide the time history of the flammable cloud with all the relevant information concerning flammable mass, flammable volume, distribution of hydrogen concentration and turbulence within the flammable cloud. For the deflagration simulation and DDT, the CFD user has to make a very sensitive decision on the time and location of ignition of the flammable cloud. Currently an agreed and validated simulation strategy that is capable to identify an ignition delay and position of ignition for the credible worst scenario does not exist. More validation experiments on ignition delay time and ignition source location are required in order to validate the CFD models and hazard/risk assessment strategy to be applied for hydrogen safety engineering.

To sum up, several current open issues exist in ignition modelling and they are considered as very critical.

Very urgent/critical issues

- Quantitative validation of CFD models.
- CFD modelling and validation of the membrane rupture and the associated transient processes, including mixing.
- CFD modelling of transition from spontaneous ignition to jet fires and/or the quenching of the spontaneous ignition.
- Development and validation of sub-grid scale models accounting for interaction of turbulence and chemistry. The required fine mesh resolutions that are used to simulate small scale experiments are not applicable yet in simulations of large real-scale configurations.
- Research and development of strategy for ignition delay time and position of ignition source for numerical simulations of deflagrations.
- Ignition in complex geometry with obstacles and some level of confinement have not been investigated enough experimentally so far.

5. FIRES

During the hydrogen release from a high pressure system, an early ignition of the flammable cloud is more likely to develop into a jet-fire rather than into a deflagration with high overpressure.

Deflagrations are modelled as premixed flames while jet fires are treated mainly as non-premixed or diffusion flames. Partially-premixed models are applied by some research groups.

According to Poinsot et al. (2005), many of the existing RANS models of turbulent non-premixed flames can be classified into two main approaches: a primitive variable method where the species mass fractions and temperature balance equations are not required and the mean reaction rates are not modelled. The conditional quantities (unknown variables) are provided from flamelet libraries or from balance equations such as in the Conditional Moment Closure or CMC model (Klimenko, 1990), (Bilger, 1993). In the reaction rate approach instead, balance equations for the species mass fraction are solved and the reaction rates have to be modelled as for turbulent premixed combustion.

A very well known LES approach for non-premixed flames is the Linear Eddy Model or LEM (Kerstein 1988, 1989, 1990, 1991, 1992), (McMurthy et al., 1992). Probability density functions can be extended from RANS to LES for species mass fraction or for reaction rates both for infinitively fast chemistry (Cook et al., 1994, 1999), (Reveillon et al., 1996) and for finite rate chemistry (Cook et al., 1998), (De Bruyn Kops et al., 1998).

Several experimental investigations of hydrogen jet fires have been performed (Blanc et al., 2009), (Gavrikov et al., 2009), (Grune et al., 2009), (Houf et al., 2007, 2009a, 2009b), (Imamura et al., 2008), (Kuznetsov et al., 2009), (Mogi et al., 2008, 2009), (Molina et al., 2007), (Proust et al., 2009) (Royle et al., 2009), (Schefer et al., 2006, 2007, 2008, 2009a, 2009b, 2009c), (Takeno et al., 2007), (Willoughby et al., 2009). The main aims of those studies are to identify the size (length and width) of the fire, the radiative properties according to the initial pressure in the tank and the outlet diameter and to investigate the effect of barriers on the fires.

Numerical simulations of jet fires from high pressure systems were performed by Zhang et al. (2007), Houf et al. (2009b), and Brennan et al. (2009).

Open issues in CFD modelling of hydrogen jet fires are:

Very urgent/critical issues

- A detailed and extensive CFD validation for large-scale H2 jet fires is missing.

- CFD reproduction of flame length/width and temperature profiles for jet fires (even under conditions of decreasing notional nozzle and H2 temperature during blowdown).

- Thermal and pressure effects of indoor hydrogen fires. The key issue to be addressed is the limit of mass flow rate from a pressure relief device that will not destroy the enclosure like garage.

- Impinging jet fires and heat transfer to structural elements, storage vessels and communication infrastructure.

- Effects of wind, surfaces, release direction, and obstacles on parameters of jet fires.

- Predictive simulations of blow-off, lift-off, and blow-out phenomena.

- Flames from plane jets (cracks).

Medium urgent/critical issues

- Combination of premixed and non-premixed cases requires further development and validation of partially-premixed models (validation of Takeno and Domingo index and of models within the Takeno/Domingo index approach)

- Self-extinction of hydrogen fires in enclosures and re-ignition.

- Dynamics of under-ventilated hydrogen jet fires in enclosures.

Less urgent/critical issues

- Modelling and simulations of micro-flames which can potentially cause domino effects. Quantitative reproduction by numerical simulations of flow rate for quenching and blow-off of micro-flames.

6. DEFLAGRATIONS

Although extensive experimental and numerical investigations of hydrogen explosions have been performed, the quantitative reproduction of experimental data by one universal CFD model is still an open issue.

Deflagrations are explosions where the flame front propagates with a subsonic speed. The range of deflagration flame speed is quite wide, from few m/s in the laminar regime to many hundreds m/s or even above 1000 m/s in the fast deflagration regime, being the hydrogen sonic speed in standard conditions equal to 1295 m/s. After ignition, the early stages of propagation of the flame are in the laminar regime. Several different physical mechanisms cause the wrinkling of the flame and the increase of the burning rate, inducing the acceleration of the flame as described in the review by Ciccarelli and Dorofeev (2008). These mechanisms include gas dynamic instabilities (Landau-Darrieus instabilities), thermal-diffusive instabilities, and in case of confinement and/or obstacles Richtmeyer-Meshkov and/or Rayleigh-Taylor instabilities, Kelvin-Helmholtz instabilities, acoustic instabilities, turbulence-chemistry interactions, etc.

By definition turbulent combustion is dominated by the turbulence-chemistry interactions. The different turbulent combustion regimes are usually represented in the Borghi diagram or regime diagram, as shown in Figure 8. The flame propagation regimes are identified in terms of the RMS velocity u', the laminar burning velocity u_L , the integral length scale l, the flame thickness δ_L, the Damköhler number Da, the Karlowitz number Ka, and the turbulent Reynolds number, Re_L.

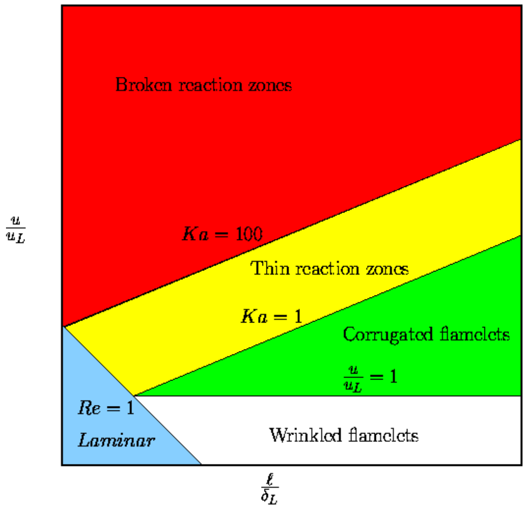

Figure 8: Regime diagram for premixed turbulent combustion regimes (Peters, 2000).

Both RANS and LES approaches require the closure of the governing equations by modelling of some terms in the equations such as the Reynolds stresses (turbulence term) and the mean source term (chemistry term) in RANS or the sub-grid stresses (turbulence term) and the filtered source term (chemistry term) in LES.

Turbulence modelling of non-reacting flows is a big issue and a huge field of investigation that will not be addressed in this report. It is sufficient to emphasize that the correct modelling of the turbulent terms is a pre-requisite for the correct modelling of the turbulent combustion problems.

Regarding the modelling of the flame front propagation, several approaches have been formulated. For RANS, they include the Eddy Break-Up or EBU (Spalding, 1971) and the Eddy Dissipation model (Magnussen and Hjertager, 1976), (Hjertager, 1982), the G-equation approach (Kerstein et al. 1988) (Peters, 1999, 2000), the Probability Density Function models such as the BML model (Bray, Moss and Libby, 1985), the Flame Surface Density models (Bray et al., 1989), (Watkins et al., 1996), and fractals models e.g. (Gouldin et al. 1989). The flame surface density can be determined also by means of a balance equation and several models exist to close that equation (Poinsot et al., 2005) such as the Cant-Pope-Bray model (Cant et al., 1990), the Coherent Flame Model (Duclos et al., 1993), the Mantel and Borghi model (1994), the Cheng and Diringer model (1991), and the Choi and Huh model (1998). Comparisons of various flame surface density models can be found in Duclos et al. (1993) and in Choi and Huh (1998).

The EBU model can be extended to a LES model by means of a sub-grid turbulent time scale (Fureby and Lofstrom, 1994) (Fureby and Moller, 1995). The modelling of the flame front propagation in LES is tackled by means of three main approaches: the artificially thickened flame approach (Butler et al., 1977), the flame front tracking approach (G-equation) (Kerstein et al. 1988) (Peters, 1999, 2000) and filtering the progress variable balance equation (Boger et al., 1998), (Knikker et al., 2002, 2004) (Weller et al., 1988) (Hawkes et al., 2000, 2001), (Molkov et al., 2005).

In the first (2005), second (2007) and third (2009) International Conference of Hydrogen Safety, numerical investigations of CFD hydrogen explosions were presented in Paillere et al. (2005), Breitung (2005), Gallego et al. (2005), Kotchourko (2005), Molkov et. al., (2005), Nozu et al. (2005), Bédard-Tremblay et al. (2007), Hansen and Middha (2007), Sommersel et al. (2007), Bauwens et al. (2009), and Rao et al. (2009, 2010).

Validation calculations of hydrogen explosions using an LES approach were performed by Molkov et al. (2006) (explosion in an empty 547-m3 vented enclosure), by Hashimoto and Matsui (2007) (explosion inside two rooms connected by a duct), by Makarov et al. (2007) (explosion in a vented spherical vessel). Venetsanos et al. carried out the RANS numerical analysis of a real-accident in a Stockholm district (Venetsanos et al., 2003) and the numerical simulations of hydrogen release and explosions in an urban district and in a tunnel (Venetsanos et al., 2007). Middha and Hansen published recently results of CFD validation of hydrogen explosions in a channel with baffles, in a vented tube, in a mock-up refuelling station and in a partial confined geometry (Middha and Hansen, 2009). In the HySafe NoE (www.hysafe.org), numerical validation exercise of hydrogen deflagrations in the open atmosphere (Garcia et al., 2010), in a refuelling station environment (Makarov et al., 2009) and in a tunnel (Baraldi et al., 2009) were performed.

One main issue in complex large scale geometry is the presence of objects with very small length scales. The geometrical representation of a hydrogen installation may contain hundreds or even thousands of objects with pipes and other elements down to dimensions of 20 mm or less. Those small objects can not be neglected in the generation of the computational mesh because they can have a significant effect on the flame surface area, and hence on deflagration development. On the other hand, a fully-resolved geometry would require an extremely fine mesh resolution that is often prohibitively expensive for the current computer resources. One approach to tackle the issue is the use of sub-grid modelling or Porosity Distributed Resistance (PDR). The PDR validation of the flow and flame interactions with the sub-grid obstacles is still an open issue.

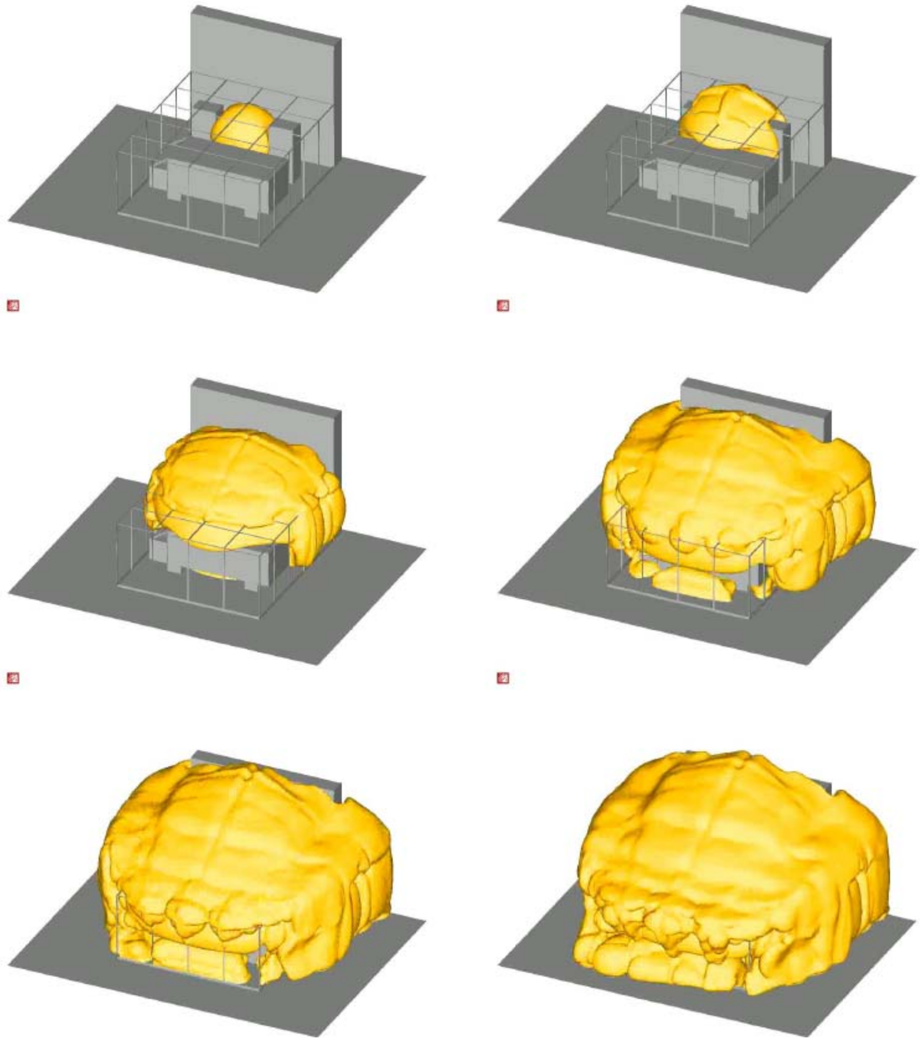

Figure 9: Flame propagation in a mock-up hydrogen refuelling station (Middha and Hansen, 2009).

Some of the main open issues in CFD modelling of deflagrations are:

Very urgent/critical issues

- Currently a single physical model and numerical tool that can cover the entire range of phenomena in flame acceleration and propagation does not exist. There are many numerical combustion models but it seems that the range of applicability of many models is limited to a specific type of event/regime.
- More experimental research is needed on laminar burning velocity for all ranges of pressure, temperature and equivalence ratio.
- The effects of thermo-diffusive instabilities, flame stretch and curvature on the flame speed are not completely understood from the quantitative point of view and in connection with numerous mechanisms affecting burning rate of hydrogen-air mixtures.
- CFD modelling and predictive simulation of all flame acceleration mechanisms or mechanisms increasing mass burning rate, including the transition between different combustion regimes such as the transition from laminar flame to turbulent regime.
- Representation of unresolved small-scale geometries in the computational mesh by physical models.
- Development of multi-phenomena combustion models that take into account mechanisms beyond an interaction between flow turbulence (intensity and scale) and combustion, e.g. Taylor instability, anisotropic effects, etc.
- Dynamics and physical mechanisms allowing to model coherent deflagrations in vented enclosures (parallel development of internal and external deflagrations). Effect of inertia of vent cover on explosion dynamics, including DDT.
- CFD validation of mitigation measures on deflagration strength e.g. appropriate use of water spray or water mist.
- CFD simulations/validation of explosions in real-scale configurations, such as complex geometry with multiple obstacles and different level of confinement.

Less urgent/critical issues

- Model constants are often adjusted in order to describe different combustion events and to enlarge artificially the range of applicability of the model. This should be clearly stated and it is expected that "varying constants" should be finally understood and explained in the scientific literature.

- Development and validation of very large eddy simulation (VLES) models and LES models in conditions of limited computer resources
- Partially premixed flames, in particular triple flames in hydrogen-air layers and their pressure effects in enclosed space.

7. DETONATIONS AND DDT

Detonations are explosions with a flame front that propagates at supersonic speed. Typically the pressure generated by a detonation is much larger than in a deflagration. Depending on mixture composition, initial conditions of pressure and temperature, and ignition energy, detonations can occur in two modes: a direct detonation where the detonation is formed instantaneously after the ignition or a transition from deflagration to detonation. In the latter case, after ignition the flame front travels at subsonic speed and later it undergoes a transition to supersonic speed through complex interactions between pressure waves, chemistry, turbulence and gas-dynamics. The onset of DDT is prompted by an explosion in an explosion and the typical situation which precedes the detonation onset is represented by a shock wave followed by a high speed subsonic deflagration. It was observed experimentally (Urtiew et al., 1966) that DDT can occur at least in four modes according to the location of the onset of detonation: at the flame front, at the shock front, between the flame and the shock front and at a contact discontinuity formed by the coalescence of two shock waves ahead of the flame. Denotations have a typical multidimensional cellular structure with incident, reflected, transverse shock waves, slip lines and triple points.

Direct detonations is in itself a very challenging phenomenon to be captured numerically but even more difficult is the transition from deflagration to detonations (DDT) because it involves different combustion regimes with different propagation mechanisms and different length scales.

Both DDT and the multi-cellular structure of detonations require an extremely fine mesh resolution of the order of microns that can be used only in small computational domains and not in real scale situations.

Many numerical works on hydrogen detonations both in 1D and in 2D have been performed (Oran et al., 1981, 1998, 1999) (Liang and Bauwens, 2005) (Radulescu et al., 2005, 2007) (Liang et al., 2007) (Bedard-Tremblay et al., 2009a) (Heidari et al., 2009). Due to the rapid growth in computational power, it became also feasible to perform simulations of the 3D multi-cellular structure of a H_2

detonation wave (Williams et al., 1996, 1997), (Tsuboi et al., 2002), (Eto et al., 2005). The resolution demands are much larger than the typical CFD resolution that can be used in real scale configurations. Since the relevant information for the risk assessment is the level of overpressures generated by the interactions of the Chapman-Jouget (CJ) pressure peak with the geometry and the obstacles, it may not be necessary to solve the multi-cellular structure of detonations. In a series of large-scale experiments on hydrogen detonations in RUT facility (310 m^3) and their 3D numerical simulation (Breitung, et al., 1994, 1996), it has been shown that simulations are able to predict 3D loads on the confining structures from *fully developed detonations* without resolution of the detonation cellular structure. It was also noted (Dorofeev, 1996a) that *marginal detonations* and cases when detonation fails and reinitiates thereafter, require sufficient resolution of cellular structure or reaction zone for prediction of the loads. For the risk assessment purposes, in many cases, capturing the flame front without cellular structure could be sufficient to determine the relevant maximum overpressures of detonations propagating in a complex geometry (Bedard-Tremblay et al., 2008, 2009b). The physics and numerics of the numerical reproduction of the von Neumann spike and detonation pressure wave on very large meshes with use of the progress variable equation and the gradient method for propagation of the reaction front of the detonation wave is presented in the recent LES model of detonation (Zbikowski et al., 2008). The last approach gives up the real thickness of detonation wave to simulate the correct pressures. A validation of a LES approach for DDT calculations can be found in Vaagsaether et al. (2007) while a RANS approach was investigated by Middha et al. (2008).

It has been shown that the CJ wave speed depends upon heat release and not on details of the kinetic model (Bedard-Trembley et al. 2009) and this allows using one-step chemistry models.

Heidari et al. (2009) developed a modelling approach for large scale hydrogen detonations. They conducted numerical simulations of the detonation tests carried out at the RUT tunnel facilities in Russia and achieved reasonably good agreement on pressure decay and the propagation speed of detonation. They also carried out predictions of planar hydrogen-air and propane-air clouds. Contrary to common belief that hot products will expand away from the centre of detonation, the predictions have revealed the existence of high negative drag impulse within the cloud. The later offers possible explanation to the directional indicators in the forensic evidence found in some major industrial accidents.

Fundamental in numerical hydrogen DDT is the work performed by Oran and coworkers (Gamezo et al., 2007, 2008), (Oran and Gamezo, 2007), (Kholkhlov et al., 1999a, 1999b) solving the Navier-Stokes equations with a one-step Arrhenius kinetics as combustion model. It must be again emphasized that the mesh resolution required to fully capture DDT can not be applied to real scale situations.

Apart from the prediction of DDT, the pressure field associated with the onset of detonations may be of interest for safety applications. It has been shown in many studies that DDT events may result in very high local overpressures. Given that the location of DDT is known or controlled by geometry (e.g. in reflection from the end-wall of a channel), the pressure field associated with DDT events may be simulated with an accuracy sufficient for engineering applications (Dorofeev, et al., 1996b).

Because of the mesh requirements and the complex physics, DDT is still one of the most challenging phenomena for CFD simulations. Probably, efforts should be concentrated on SGS modelling of DDT on coarse computational grids relevant to industrial scales.

Open issues in detonation and DDT are:

Very urgent/critical issues

- Development of models and quantitative reproduction of experimental data by CFD.
- Very high mesh resolution requirements or reliable SGS models of DDT.
- Simulations of pressure and impulse dynamics in real-scale complex geometries.

Medium urgent/critical issues

- Real gas properties and gas law.

8. ACCIDENT CONSEQUENCES

Combustion of hydrogen can be a reason for adverse pressure and thermal effects on people and surroundings. Explosions can cause damages to people, equipment and buildings due to the generated overpressures/impulse and to the flying debris (the so-called missile effect) while for fires the main safety concern is due to the heat fluxes.

IEA Hydrogen Implementing Agreement (HIA) Task 19 on hydrogen safety has been developing recommendations for uniform harm criteria to be used in the quantitative risk analysis of the hydrogen infrastructure. These recommendations, presented at ICHS3 in Ajaccio in September 2009 (LaChance et al., 2009), provide a comprehensive analysis of available engineering models (Probit functions) that allow the user to predict thermal and pressure effects associated with unwanted events and provide rationale for selection of the models most appropriate for hydrogen. It needs to be noted here that the Probit functions shown below are generic and, thus, their validation for hydrogen is essential. CFD can play a critical role in this regard.

The final aim of the CFD analysis performed for risk assessments is the estimate of the level of the relevant parameters (overpressures, impulse, heat fluxes) in the region of the accidental event and its surroundings. From the distribution of those parameters in the accident region, it is possible to correlate the level of damages with the distance from the location of the explosions or the jet fires, identifying safety distances.

Damage criteria can be defined as in Table 2 and Table 3 for the heat fluxes and Table 5 for the overpressures. The most widely used methodology to determine damages and take into account the heterogeneity in the response of the exposed population to the same dangerous phenomenon is based on the Probit equations (Ferradas et a., 2008). By means of the Probit equations, a statistical correlation between the magnitudes of the danger (overpressure, impulse, heat fluxes, weight and speed of the flying debris) and the percentage of the population affected is defined. Probit equations for damages due to radiation are shown in Table 4 while the Probit equations for harm due to overpressure/impulse and to the missile effect are listed in Table 6. As shown in the tables, there is not a unique Probit equation that is universally accepted. In Figure 10 and Figure 11, the Probit equations for heat fluxes and overpressure are illustrated and it must be emphasized that there is a certain level of scattering on the graph.

Physically underpinned and well validated CFD codes can provide relevant information about the pressure and the radiation field for the Probit correlations. For the missile effect, a relatively new area, FSI fluid-structure interaction, is developing quickly in order to describe the structural failure, the subsequent fragmentation of the structure and the flying debris in case of TNT explosions (Casadei, 2008), (Giannopoulos et al., 2010). Nevertheless FSI has not been validated so far.

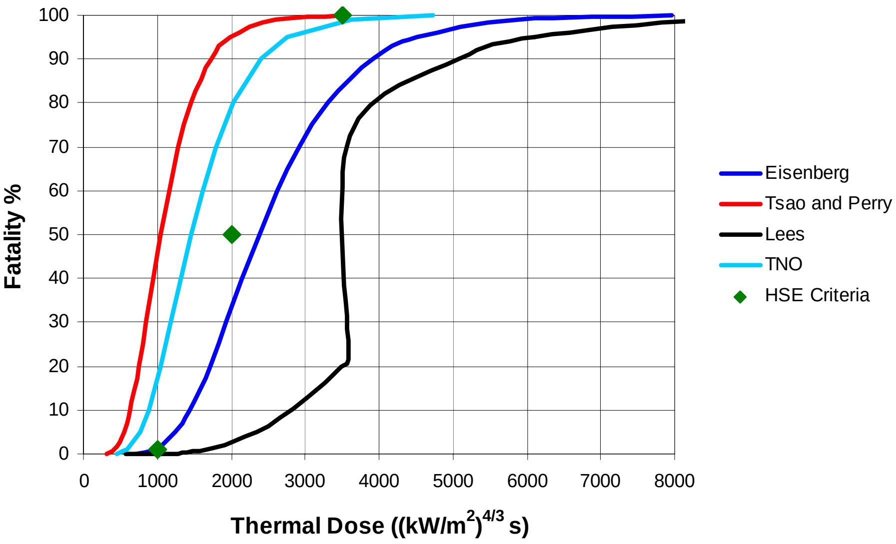

Figure 10: Thermal dose versus fatalities according to different Probit equations.

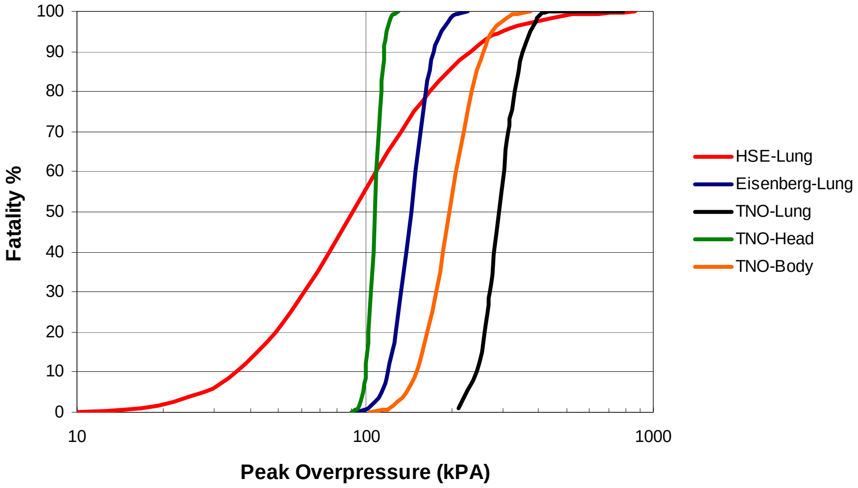

Figure 11: Overpressure versus fatalities according to different Probit equations.

Table 2: Harm criteria for heat fluxes to people (World Bank, 1988).

Thermal Radiation (kW/m2)	**Type of Damage**
1.6	No harm for long exposures
4 to 5	Pain for 20 second exposure; first degree burn
9.5	Second degree burn after 20 seconds
12.5 to 15	First degree burn after 10 seconds; 1% lethality in 1 minute
25	Significant injury in 10 seconds; 100% lethality in 1 minute
35 to 37.5	1% lethality in 10 seconds

Table 3: Threshold doses for radiation burn (Pew, 1997).

Burn Severity	**Threshold Dose (kW/m2)$^{4/3}$s**	
	Ultraviolet	Infrared
First Degree	260-440	80-130
Second Degree	670-1100	240-730
Third Degree	1220-3100	870-2640

Table 4: Thermal dose Probit functions for human response.

Reference	**Probit Equation**	**Comment**
First Degree Burn		
TNO, 1989	$Y = -39.83+3.0186 \ln [V_1]^1$	Based on Eisenberg model but accounts for infrared radiation.
Second Degree Burn		
TNO, 1989	$Y = -43.14+3.0186 \ln [V_1]^a$	Based on Eisenberg model but accounts for infrared radiation
Fatality		
Eisenberg, 1975	$Y = -38.48 + 2.56 \ln [V_1]^a$	Based on nuclear data from and (ultraviolet radiation)
Tsao et al., 1979	$Y = -36.38 + 2.56 \ln [V_1]^a$	Eisenberg model modified to account for infrared (2.23 factor)
TNO, 1989	$Y = -37.23 + 2.56 \ln [V_1]^a$	Tsao and Perry model modified to account for clothing (14%)
Lees, 1994	$Y = -29.02 + 1.99 \ln [V_2]^b$	Accounts for clothing, based on porcine skin experiments using ultraviolet source to determine skin damage, uses burn mortality information

[a] V_1 = I4/3t = thermal dose in (W/m2)$^{4/3}$s.

[b] V_2 = F*I4/3t = thermal dose in (W/m2)$^{4/3}$s where F=0.5 for normally clothed population and F=1.0 when clothing ignition occurs.

Table 5: Damage to humans, structures and equipment due to overpressures.

Overpressure (kPa)	Description of Damage
Direct Effects on People (Jeffries et al., 1997)	
13.8	Threshold for eardrum rupture
34.5 to 48.3	50% probability of eardrum rupture
68.9 to 103.4	90% probability of eardrum rupture
82.7 to 103.4	Threshold for lung hemorrhage
137.9 to 172.4	50% probability of fatality from lung hemorrhage
206.8 to 241.3	90% probability of fatality from lung hemorrhage
48.3	Threshold of internal injuries by blast
482.6 to 1379	Immediate blast fatalities
Indirect Effects on People (Jeffries et al., 1997)	
10.3 to 20.0	People knocked down by pressure wave
13.8	Possible fatality by being projected against obstacles
55.2 to 110.3	People standing up will be thrown a distance
6.9-13.8	Threshold of skin lacerations by missiles
27.6 to 34.5	50% probability of fatality from missile wounds
48.3 to 68.9	100% probability of fatality from missile wounds
Effects on Structures and Equipment (Guidelines, 1998)	
1	Threshold for glass breakage
15-20	Collapse of unreinforced concrete or cinderblock walls
20 to 30	Collapse of industrial steel frame structure
35 to 40	Displacement of pipe bridge, breakage of piping
70	Total destruction of buildings; heavy machinery damaged
50 to 100	Displacement of cylindrical storage tank, failure of pipes

Table 6: Probit functions for damage caused by overpressure.

Probit	Probit Equation	Application
Human Fatality		
AICHE, 1998, 2000	$Y = -77.1 + 6.91 \ln [Ps]$[a]	Death due to lung hemorrhage
HSE (1991)	$Y = 1.47 + 1.371 \ln [Ps]$[a]	Death due to lung hemorrhage
TNO (1989)	$Y = 5 - 5.74 \ln [4.2\, Po/Pef + 1.3/isc]$[b]	Death due to lung hemorrhage
TNO (1989)	$Y = 5 - 8.49 \ln [2430/Ps + 4x10^8/Psi]$[c]	Death due to head impact
TNO (1989)	$Y = 5 - 2.44 \ln [7380/Ps + 1.3x10^9/Psi]$[c]	Death due to whole body impact
TNO (1989)	$Y = -13.19 + 10.54 \ln [vo]$[d]	Death due to fragments > 4.5 kg
TNO (1989)	$Y = -17.56 + 5.3 \ln[S_1]$[e]	Death due to fragment masses of 0.1 to 4.5 kg
TNO (1989)	$Y = -29.15 + 2.1 \ln[S_2]$[f]	Death due to fragments masses of 0.001 to 0.1 kg
Structure Failure		
AICHE, 1998, 2000	$Y = -23.8 + 2.92 \ln [Ps]$[a]	Total damage
TNO (1989)	$Y = 5 - 0.26 \ln[V_1]$[g]	Minor damage
TNO (1989)	$Y = 5 - 0.26 \ln[V_2]$[h]	Major damage
TNO (1989)	$Y = 5 - 0.22 \ln[V_3]$[i]	Collapse

[a] P_s = peak overpressure in Pa

[b] P_o = atmospheric pressure in Pa, $i_{sc} = i/(P_o^{1/2}\, m^{1/3})$, m = mass of person in kg, $P_{ef} = P_s + 5P_s^2/(2P_s + 1.4x10^6)$, and P_s = peak overpressure in Pa

[c] P_s = peak overpressure in Pa, i = impulse of the shock wave (Pa*s)

[d] v_o = debris velocity in m/s

[e] $S_1 = 0.5 * m * v_o^2$, m = debris mass in kg, v_o = debris velocity in m/s

[f] $S_2 = m * v_o^{5.115}$, m = debris mass in kg, v_o = debris velocity in m/s

[g] $V_1 = (4600/P_s)^{3.9} + (110/i)^{5.0}$, P_s = peak overpressure in Pa, i = impulse of the shock wave in (Pa*s)

[h] $V_2 = (17500/P_s)^{8.4} + (290/i)^{9.3}$, P_s = peak overpressure in Pa, i = impulse of the shock wave (Pa*s)

[i] $V_3 = (40000/P_S)^{7.4} + (460/i)^{11.3}$, P_S = peak overpressure in Pa, i = impulse of the shock wave (Pa*s)

9. CONCLUSIONS

The report describes the findings of a workshop that was held at the Institute for Energy (JRC) in Petten Netherlands, on the topic “Gap analysis of CFD modelling of hydrogen release and combustion”. The main topic was divided in 6 sub-topics: release and dispersion, auto-ignition, fires, deflagrations, detonations and DDT, and accident consequences.

For each sub-topic, the main gaps in CFD modelling were identified and prioritised. Further development/validation of CFD code(s) for simulations of hydrogen safety related phenomena is a general issue that affects all sub-topics.

It must be emphasized that a model evaluation protocol for CFD applications for hydrogen safety, as the one developed for LNG dispersion (Ivings et al., 2007, 2008), does not exist. In order to apply CFD with full confidence in the accuracy of the simulations results, for each hydrogen sub-topic a validation protocol or model evaluation protocol should be developed. The benchmarking activities of the protocol should be based on a matrix of experiments. Carrying out new experiments may be necessary, at least for some sub-topics, in order to assure that the matrix covers all the relevant aspects of the physical phenomena. The protocol will be the procedural tool to identify the more suitable models for each sub-topic and to define the level of uncertainties for all the tested models/codes.

Moreover the protocol could work as a catalyst to accelerate both the improvements of existing codes and models and the developments of new models/codes with increased predictive capabilities.

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Abstract

The report describes the findings of a workshop that was held at the Institute for Energy (JRC) in Petten Netherlands, on the topic “Gap analysis of CFD modelling of hydrogen release and combustion”. The main topic was divided in 6 sub-topics: release and dispersion, auto-ignition, fires, deflagrations, detonations and DDT, and accident consequences. For each sub-topic, the main gaps in CFD modelling were identified and prioritised.

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