STATE OF THE ART AND RESEARCH PRIORITIES IN HYDROGEN SAFETY

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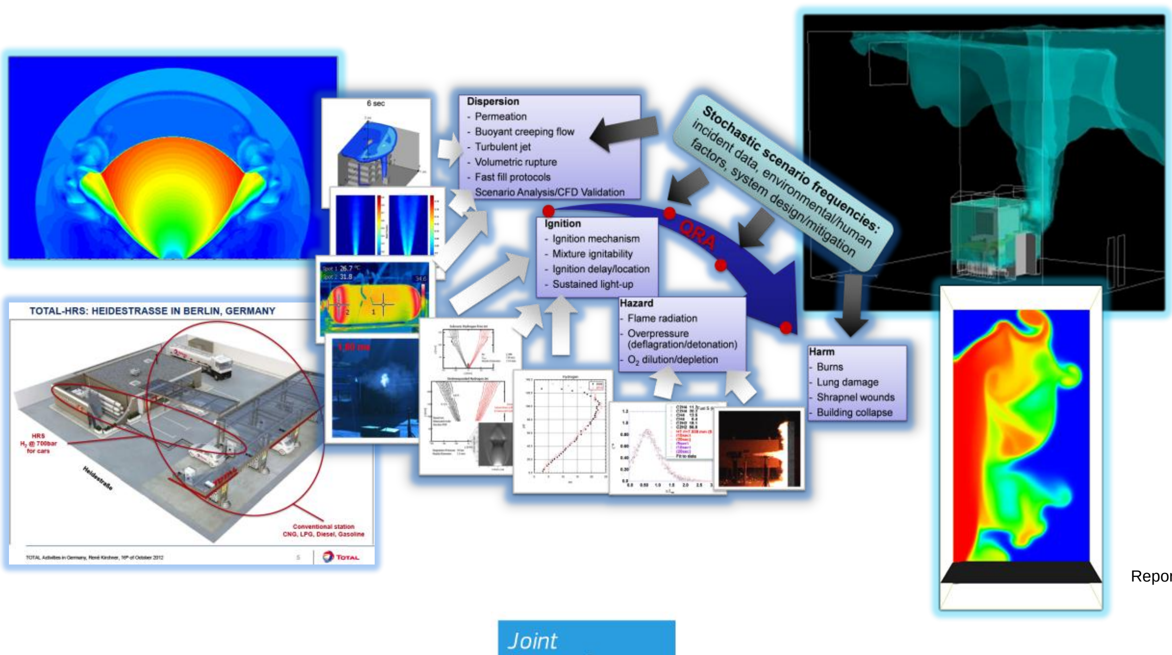

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EXECUTIVE SUMMARY

SETTING THE STAGE

Preamble

The International Association for Hydrogen Safety (HySafe) strives to be the main global forum for hydrogen safety related issues. It is an international non-profit organization that currently has more than 30 members from industry, research organizations and universities representing 14 countries worldwide[1].

The Association facilitates the networking for the further development and dissemination of knowledge and for the coordination of research activities in the field of hydrogen safety. IA HySafe experts collaborate to assess the state of-the-art in hydrogen safety approaches and assessments and to identify and prioritise topics for further hydrogen safety research to be fed into the strategic agenda of hydrogen technology research and innovation programmes worldwide.

The Institute for Energy and Transport (IET) of the Joint Research Centre (JRC) of the European Commission provides scientific and technical support on energy and transport issues to policy makers of the European Union (EU). One of IET's key scientific activities is Hydrogen Safety in Storage and Transport, which supports the safe and cost-effective market penetration of hydrogen as an alternative fuel in vehicles and as an energy storage medium for renewable energy systems.

Although fuel cells and hydrogen technologies have not fully penetrated the market yet, industry has already identified applications that exploit one or more advantages of the technology (high efficiency and associated reduced energy consumption, low noise, low heat signature, absence of exhaust fumes, reduction of space requirements and weight, lower maintenance requirements, etc.) and has implemented these using current technology. Examples include material-handling vehicles, back-up and UPS stationary power, portable applications, vehicle auxiliary power units, captive fleets and scooters/wheelchairs. For example, in North America within the last 5 years thousands of hydrogen fuel cells systems have been deployed for materials handling (predominantly), back-up power and combined heat and power (CHP) applications, with Japan, Korea and EU following suit.

However, while fuel cells and hydrogen technologies are already penetrating the market in a number of applications, sustained R&D, private and public, is still needed for effectively addressing the remaining high-risk technological barriers in a pre-competitive environment. One of the key R&D areas, preferably to be carried out through international cooperation, is pre-normative research for the establishment of fit-for-purpose Regulations, Codes and Standards (RCS) to ensure fuel cells and hydrogen technologies are deployed safely.

The EU dimension: Horizon 2020

In regard to standards development and safety, COM(2011)809 - Proposal for a Regulation of the European Parliament and of the Council establishing Horizon 2020, the European Union Framework Programme for Research and Innovation (2014-2020) - notes that activities in

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[1] Canada, Denmark, France, Germany, Greece, Italy, Japan, Netherlands, Norway, Poland, Russia, Spain, United Kingdom and United States

support of **standardisation** and interoperability, **safety and pre-regulatory activities will be promoted.** The direction given to JRC in this regard is to focus on European Union policy priorities while **enhancing cross-cutting competences. Energy, transport and safety are listed among JRC's key priorities for pre-normative research.**

The Proposal for a Council Decision establishing the Specific Programme Implementing Horizon 2020 COM (2011)808, stresses that **international cooperation** with third countries is necessary to address effectively the societal challenges defined in **Horizon 2020**. In particular, development of **worldwide standards and guidelines** is identified as a major enabler to increase competitiveness of industry.

IA HySafe has a unique structure that includes a **research committee** attending to the state-of-the-art research in hydrogen safety, an **industry relations committee** attending to the needs of industrial stakeholders both in hydrogen safety and standardization, a **public relations and knowledge dissemination committee** attending to outreach and educational and training needs of various stakeholders, and a **conference committee** that leads the scientific organization of the only **International Conference on Hydrogen Safety**. This structure makes HySafe an ideal partner to collaborate with JRC IET within the EU and with other entities worldwide to identify R&I safety priorities and address them though its members. In the context of the EU, HySafe and JRC-IET support the European Fuel Cell and Hydrogen Joint Undertaking (FCH-JU) by providing the scientific and technical basis for safety-related standardization and regulation.

PRIORITIZATION OF RESEARCH AND DEVELOPMENT IN HYDROGEN SAFETY

Wide spread deployment and use of hydrogen and fuel cell technologies can occur only if hydrogen safety issues have been addressed in order to ensure that hydrogen fuel presents the same or lower level of hazards and associated risk compared to conventional fuel technologies. To achieve this goal, hydrogen safety research should be directed to address the remaining knowledge gaps using risk-informed approaches to develop engineering solutions and Regulation Codes and Standards (RCS) requirements that meet individual and societal risk acceptance criteria, yet are cost-effective and market-competitive.

Identification of the state-of-the-art and of research priorities is best conducted in consultation with a group of experts representing industry and research organizations.

Building on the success of the previous workshop organized by JRC IET in October 2009 to address knowledge gaps in CFD modelling (JRC Reference Reports 2011), HySafe and JRC IET partnered to organize a Research Priorities Workshop in Berlin on October 16-17, 2012 hosted by BAM. The participating experts were carefully selected among the HySafe members and JRC according to their experience/expertise, number of scientific publications and participations in International Conferences, seminars, workshops as well international and European funded projects.

By performing a consultation with industry and a broader research community as well as a state of the art review on hydrogen safety issues (including of CFD modelling), a consensus was reached among the experts as to the remaining gaps in the field and on the priority of the research needs. This report presents the findings and recommendations of the workshop and subsequent discussions among the participants.

Potential Impact

Identifying the remaining knowledge gaps is a logical and necessary step for making decisions on the next steps to ensure the full and safe utilization of hydrogen. This manuscript aims to become a reference document for researchers/scientists and technical (including industry) experts working in the area worldwide. HySafe and JRC-IET hope the report will serve and benefit the European Fuel Cell and Hydrogen Joint Undertaking and other funding bodies/organizations worldwide that must make decisions on research programmes and on the selection of projects to be financially supported. The performed analysis and ensuing recommendations will work as a catalyst to accelerate the improvements of existing research programmes and the developments of new engineering guidelines and industrial practices, as well as supporting the formulation of and compliance with RCS requirements.

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1. INDUSTRY PERSPECTIVE

EXECUTIVE SUMMARY

Consultations with industry stakeholders constitute a critical component in setting research priorities. From this perspective, breadth of industry representation is important. For this reason, the companies operating within different market segments of the hydrogen and fuel cell sector were invited to share their experiences and needs as well their perspectives on research priorities in the field of hydrogen safety and standardization. The industry perspective was presented from four different market segments as follows:

- Hydrogen fuel cells developer and provider – Ballard Power Systems, Canada
- Global industrial gas company – Air Liquide, France
- International fuel and refuelling provider – Total, Germany
- Multi-industrial corporation – Kawasaki Heavy Industries, Japan

A common theme in the industry message was articulated by Air Liquide was to improve knowledge quality for practical applications. This can be achieved by

- Prioritizing knowledge gaps
- Focusing research on industry needs
- Efficient dissemination channels for research findings to industry and standard development organisations (SDO)
- Aiming towards international collaboration, standardization and shared guidelines.

In reviewing industry views presented by Ballard (Jake DeVaal) and Air Liquide (Sidonie Ruban) it is remarkable to note that Air Liquide's first markets (e.g., telecom backup, mobile generators, forklifts, and automotive) all appear highly similar to Ballard's chosen markets. This suggests that the adoption of fuel cell technologies in the market place treads along the growth of their value propositions in these various applications one-by-one. In terms of the new safety challenges that Air Liquide identifies, (e.g., leak tightness, material compatibility, containment of high pressure, inherently safer 'indoor' use, and the need to understand failure mechanisms for mobile composite storage especially in fire conditions), these are common issues that Ballard shares an interest in, especially in its system products; but, due to fuel containment issues typically being the responsibility of the gas supplier or tank manufacturer, the fuel cell industry has typically avoided these, but has addressed some aspects of indoor operation as part of understanding leak outcomes behaviour (SAE Paper: 2007-01-0437).

A similar situation exists for the industry perspectives on H_2 refuelling stations (from René Kirchner, Total Germany) and on large-scale LH2 infrastructure (from Suguru Oyama and Shoji Kamiya, KHI), where the determination of safety distances, regulator/certification involvement in permitting these installations, and, most important, public acceptance of these are the main common themes shared across the diverse industry perspectives. Thus, while each industry tends to come with its own set of barriers and specific challenges, the common thread is the need to understand how hydrogen in production, storage, delivery, and use systems behaves under leak or emission conditions, and measures needed so that failures in these systems, although unlikely, will not pose undue risks to users or the public. The workshop confirmed that closer collaboration between hydrogen industry and research organisations is needed for knowledge transfer, e.g. in further reduction of separation distances through optimisation of piping diameters, hydrogen mass flow rates, etc. This could be achieved through an establishment of international educational programme to which hydrogen industry and international/national projects would have to have systematic access by delegating their experts.

Ballard Power Systems, Canada

Ballard Power Systems Inc. was founded in 1979, under the name "Ballard Research Inc.", to conduct research and development on high-energy lithium batteries. In the course of investigating environmentally clean energy systems with commercial potential, the Company began developing proton exchange membrane (PEM) fuel cells in 1983.

Proof-of-concept fuel cells followed shortly thereafter and, from 1992 to 1994, sub-scale and full-scale prototype systems were developed to demonstrate the technology.

By the early 2000's Ballard was a dominant player in automotive fuel cell development, with Ballard stacks used in Daimler and Ford automotive demonstration programs, and also in the very successful European CUTE bus demonstration project. Based on the progress made in developing several generations of automotive fuel cells, it was recognized that the investment required to develop a commercially-viable automotive fuel cell stack would exceed the company's resources, and the decision was taken in January 2008 to divest the automotive stack development assets to Daimler AG and Ford Motor Company and a newly created private company, AFCC, Auto Fuel Cell Cooperation Corp.

With the sale of Ballard's automotive stack development team to the OEMs the company's strategic focus shifted from long-term, high cost automotive fuel cell technology development to clean energy fuel cell products for near-term commercial markets. The applications that Ballard chose to shift its focus to in its drive to become profitable were fuel cell systems for buses, stacks for material handling (forklifts) and backup power (for telecom), and systems for distributed generation of electricity (MW-level stationary).

Different applications for PEM fuel cells have different lifetime and reliability requirements and expectations, where fuel cells used in backup power applications typically only require about 2500 to 4000 hours of continuous life, but require a high reliability to generate rated-power when called upon. Forklifts using Ballard PEM technology can currently achieve about 8000 to 12,000 hours of operation, while automotive stacks require and typically last about 5,000 hours, whereas buses (as potential replacements for diesel engines) require more than double this (~12,000 hours).

The business case for using fuel cells in different applications is primarily dependent on: 1) the perceived-value associated with the use of zero-emission technology, 2) the current high-cost of fuel cells, and 3) the costs of implementing these systems relative to the costs of the technology being displaced. By way of example, to date, the use of zero-emission fuel cells in forklifts has assisted in their adoption (relative to CNG or propane), but the primary basis for their adoption has been that they have proven cost-effective relative to systems.

For fuel cell powered buses, the primary advantages are zero-emission operation and reduced noise and vibration, while providing high torque and comfort to passengers. The barriers to commercialization are: 1) high initial cost (~2-3x a diesel bus), 2) higher fuel cost (~1.4 to 1.8x diesel, even though the cells are ~1.8x more efficient), and higher maintenance costs (~1.8x diesel).

A similar situation exists for Distributed Generation (DG), where the drivers for adoption include: 1) availability of by-product hydrogen (at present ~15% of all by-product H_2 produced is vented or burned), 2) feed-in tariff programs or high electricity costs (e.g., Self-Generation Incentive Programs (SGIP), and 3) governmental capital incentive purchase programs for fuel cells. Barriers to commercialization, on the other hand (as shown in Figure x), include: 1) no clear definition of what a DG plant is (e.g., is it a stationary power plant, a back-up power generator, or a peaking plant used to supplement high grid use), 2) high capital costs; long delivery and cashflow issues with high costs to certify and site these plants, and 3) risk-averse large chemical company or utility customers, who insist on proof of durability and safety, and cost-recovery up-front before purchasing a plant.

With these noted advantages and barriers to commercialization for Bus and DG products, Ballard is continuing to work to lower fuel cell costs, and has identified the following specific areas for near-term hydrogen safety research:

- Improved fuel flow monitoring for hydrogen leak detection in Bus and DG products,
- Tools and approaches for addressing the H_2/N_2 start-up discharge-emission hazard,
- Improved understanding of fuel cell recombination effectiveness, where recycling leaked H_2 through stacks is highly effective at recombining fuel but can also cause crossover leaks,
- Improved understanding of cathode air filtration effectiveness and H_2 fuel quality issues (e.g., biogas quality), and
- Qualify/use risk analysis tools and develop more meaningful standards.

Figure 1. Commercialization Barriers for MW-level Distributed Generation Power Plants

Air Liquide, France

Air Liquide is a world leader in gases for industry, health and environment. It has a long experience in the sector: more than 40 years in the hydrogen field and 10 years in fuel cells development and deployment. Air Liquide acquired vast experience in the "hydrogen chain" that includes production, storage, distribution as well as dispensing via hydrogen stations. Through the years Air Liquide built globally an infrastructure that includes more than 200 hydrogen production plants and a broad range of hydrogen distribution assets such as pipelines (more than 1,850 km), trucks and cylinders.

Overall, Air Liquide's global hydrogen production capacity is over 9 billion Nm^3 (normal cubic meter) per year (2010) with 55 hydrogen stations deployed.

Air Liquide is actively involved in commercialization of hydrogen energy applications such as materials handling (forklifts), mobile generators, telecommunications (remote sites) and mobility (such as vehicles and buses refuelling). To meet customers' expectations, high-reliability systems are being developed with competitive TCO (total cost objectives) targets.

In the telecommunications market segment the focus is on stationary fuel cells with an average electric power of 0.1 to 3 kW, mainly for substituting diesel generators (for off-grid power supply and for backup power). Hydrogen is supplied and stored in cylinder bundles under pressure between 20 and 70 MPa. Air Liquide provides full service including telemonitoring, maintenance and hydrogen storage management.

In distributed and decentralized energy market segment the focus is on hydrogen generation and storage, and electricity delivery at the right time and place. Areva presented by its part (Helion) is Air Liquide's partner in H2E project. They have developed a fuel cell-based back up power system up to 100 kW; a PEM electrolyser for industrial and energy applications with the range between 10 and 100 Nm^3/hour; a hydrogen-based storage system to address renewable energy sources intermittency, power distribution networks support, especially in developing countries (GreenergyBox™ technology).

In the materials handling market segment the focus is on hydrogen supply and refuelling of fuel cell forklifts. Hydrogen is either produced on site or delivered via tube trailers as a compressed gas or in liquid form by LH_2 tankers.

To develop a sustainable mobility with hydrogen one needs to develop a dedicated refuelling infrastructure. This task, in turn, is faced with a number of challenges, in addition to the safety-related ones:

- Hydrogen production must be
  - Based on clean (preferably) renewable technologies (carbon free or at least neutral)
  - Both centralized and distributed
  - Cost competitive
- Hydrogen transport and distribution must be
  - Efficient
  - Optimized for logistics options
  - Cost competitive
- Hydrogen storage must be
  - High capacity
  - Efficiently packaged
  - Cost competitive
- Hydrogen use in fuel cells faces challenges of
  - Fuel quality
  - Performance

    - Durability
    - Cost competitiveness
- Social acceptance is absolutely critical for deep market penetration. It should be based on shared safety knowledge and adoption of practical codes & standards.

From this perspective it is important to develop complete and optimal supply chains that will include hydrogen production, storage and distribution as well as local electricity production. These new supply chains will be based on innovative technologies developed with the joined effort of R&D and safety studies at a competitive market cost.

Air Liquide had been following this logic model via demonstration projects with prototypes and gradually developing competitive products. The examples are many: through its subsidiaries like Axane, HyPulsion and in collaboration with partners like Composites Aquitaine and Helion, Air Liquide developed products in air and oxygen PEM fuel cells, PEM electrolysers, hydrogen distribution systems, high pressure mobile storage system and refuelling systems for materials handling.

Since the start of Hydrogen Horizon Energy (H2E) project in 2009, by end of 2011 the partners deployed 97 hydrogen and fuel cells systems, filed 30 patent applications and declared 43 inventions, increased systems reliability from 91.2 to 99.2%, while achieving TCO reduction.

Next steps for 2012 – 2014 timeframe include:

- Reaching 8,000 hours milestone for PEM FC field operation (2012)
- Deployment of PEM electrolyser and fuel cell for solar energy storage (2012)
- Homologation of 52.5 MPa composite cylinders for hydrogen storage for material handling equipment (MHE) (2013)
- Approval of 5.25 MPa cylinder dispensing station for MHE (2013)
- New Axane modular fuel cell deployment to markets in Europe and Asia (2013)
- Deployment of Helion back up power systems for critical equipment (2013)
- Deployment of 5.25 MPa systems for material handling operations in Europe (2014)
- Deployment of stationary systems in East Europe and Asia (2014)
- Meeting cost reduction target for hydrogen distribution station (2014)
- Project launch for Blue Hydrogen production via PEM electrolysis (2014)

These new activities create new safety challenges such as:

- High pressure and specific mechanical loading
    - Leak tightness
    - Material compatibility (incl. hydrogen embrittlement)
    - Intelligent depressurizing tap
- "Indoor" use (enclosed environment):
    - Natural ventilation
    - Structural strength of enclosures
- High capacity of hydrogen mobile composite storage
    - Failure mechanisms
    - Fire resistance

In the past few years a number of knowledge gaps have been closed such as:

- Considering pipeline steel microstructure and fatigue enhanced embrittlement in addition to material composition (Stalheim, et al., 2008)
- Sizing release flow rate for fire protection of hydrogen composite cylinder taking into account pressure peaking effect, flame effects and storage leak and no burst phenomena (Ruban, et al., 2011)

- Sizing openings for an efficient natural ventilation of enclosures: parameters such as opening size and position which have a strong influence on dispersion regimes

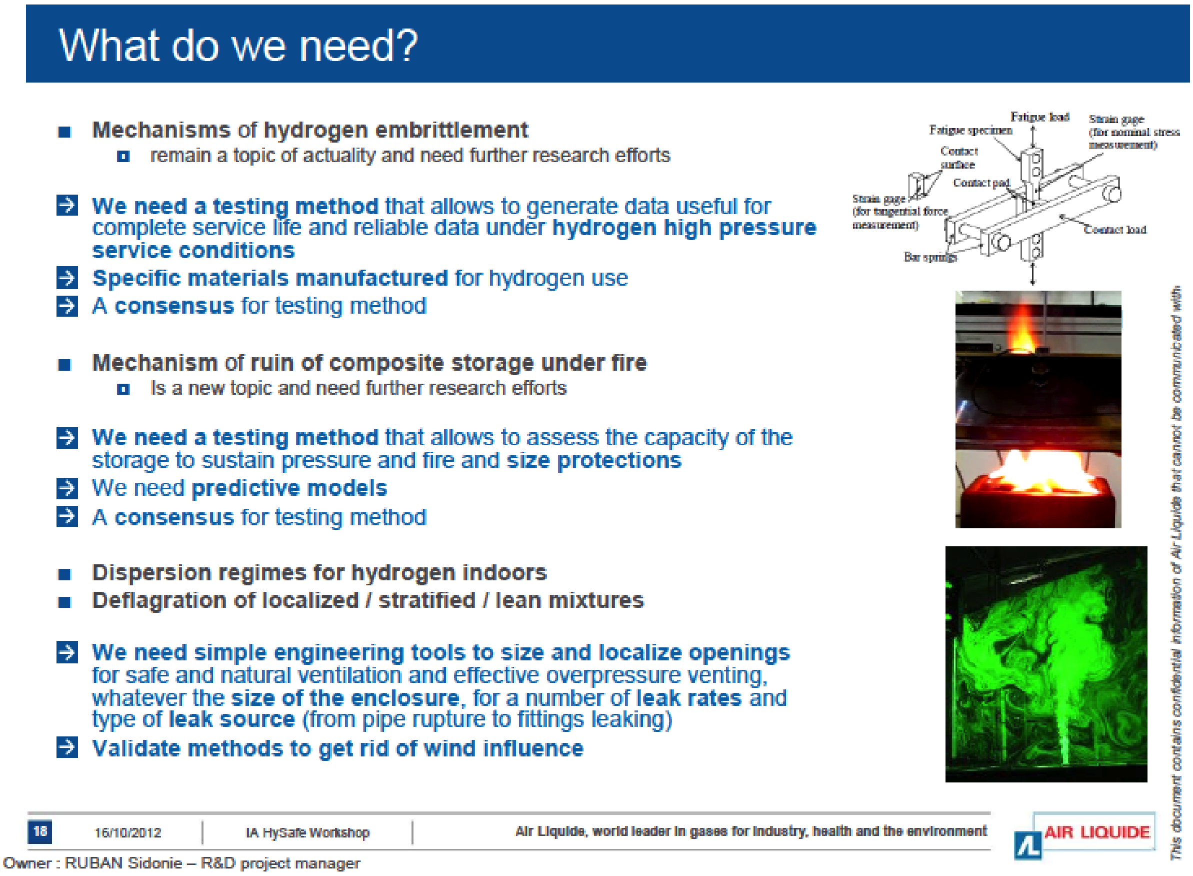

Figure 2. Research priorities as per Air Liquide needs.

Total Germany, Hydrogen / E-Mobility

Total Germany started hydrogen activities in 2002 with a first station delivering gaseous hydrogen to the BVG buses (Berlin public transport authority). Since that time Total Germany acquired experience in hydrogen refuelling via 7 more hydrogen refuelling stations (HRS) projects including its first public hydrogen dispensing combined with a conventional station in Berlin in 2006. This was followed by another HRS in Berlin in 2011 where hydrogen refuelling was integrated into a new design with other fuels like CNG, gasoline, diesel and LPG. Total Germany has also acquired significant experience with HRS permitting process.

The past 10 years were an invaluable learning experience for Total Germany that allowed to:

- Perform analysis and evaluation of distribution technologies and operation of Hydrogen Refuelling Stations (HRS) such as:
  - Monitor technology
  - Contribute to technical improvements
  - Gain experience through day-by-day operation of HRS to increase internal know-how
  - Evaluate cost structure (CAPEX and OPEX)
  - Study consumers behaviour (customers expectation)
- Create and/or improve relationships with automobile OEMs

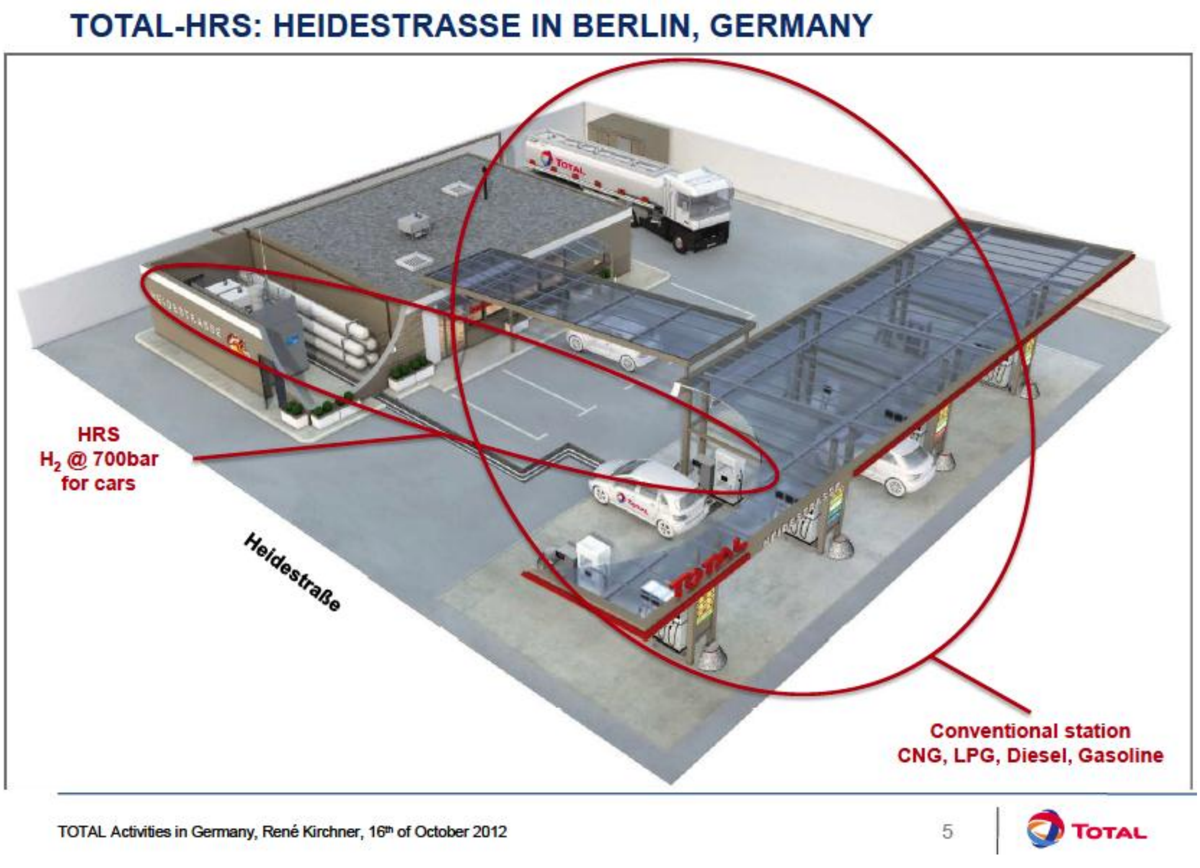

Figure 3. Configuration of Total HRS in Berlin.

During multiple permitting processes Total Germany developed excellent collaboration with TÜV (Technical Inspection Agency). It also transferred a lot of know-how on HRS to local authorities in Berlin. In this regard, close communication with local authorities before submitting a formal application was critical. It should be noted that integration of HRS into a conventional business model of a refuelling station shortened an application process.

Specific Total's learning experience:

- Local authorities need to be informed and involved as much and as early as possible

- Need for an overall guideline for HRS permitting (DIN, EN or ISO) to feel comfortable with and accelerate the process
- Knowledge dissemination within local authorities in Germany is inevitable and needed
- Exchange of experience within industry (CEP is a good example)
- Key open issues as barriers to HRS commercialization:
- Hydrogen metering
- Hydrogen quality sampling
- Refuelling protocol, particularly for 70 MPa dispensing.

Kawasaki Heavy Industries, Japan

Founded in 1878, Kawasaki Heavy Industries, Ltd. (KHI), is a leading global diversified manufacturer of transportation equipment and industrial goods. With a broad technological base that encompasses land, sea, and air applications, the KHI Group manufactures ships, rolling stock, aircraft and jet engines, gas turbine power generators, environmental and industrial plants, and a wide range of manufacturing equipment and systems. KHI also produces world-famous consumer products such as motorcycles and personal watercraft.

As per current (2013) breakdown of Japan's energy supply, 9% comes from renewable energy sources and 26% - from nuclear. New energy and environmental strategy of Japan announced in September 2012 aims to lowering nation's reliance on nuclear energy to zero within 2030s. This goal puts a lot of pressure on developing zero emission energy sources besides nuclear. Hydrogen energy based on CO_2 free hydrogen production is viewed as one of key energy vectors of the future in Japan.

Hydrogen sources are viewed to be derived from either renewable energy (solar and wind via water electrolysis) and fossil sources with carbon capture and sequestration (CCS) at a production site, even when outside Japan. In view of that, the KHI Group is directing concerted effort into the realization of a CO2-free hydrogen chain concept in pursuit of both CO2 reduction and stable energy supply. As a first step, KHI aims to build a small-scale demonstration chain and is pursuing activities, mainly R&D and feasibility studies on the concept while working with outside partners, including Japanese and Australian government agencies and leading companies that run hydrogen businesses.

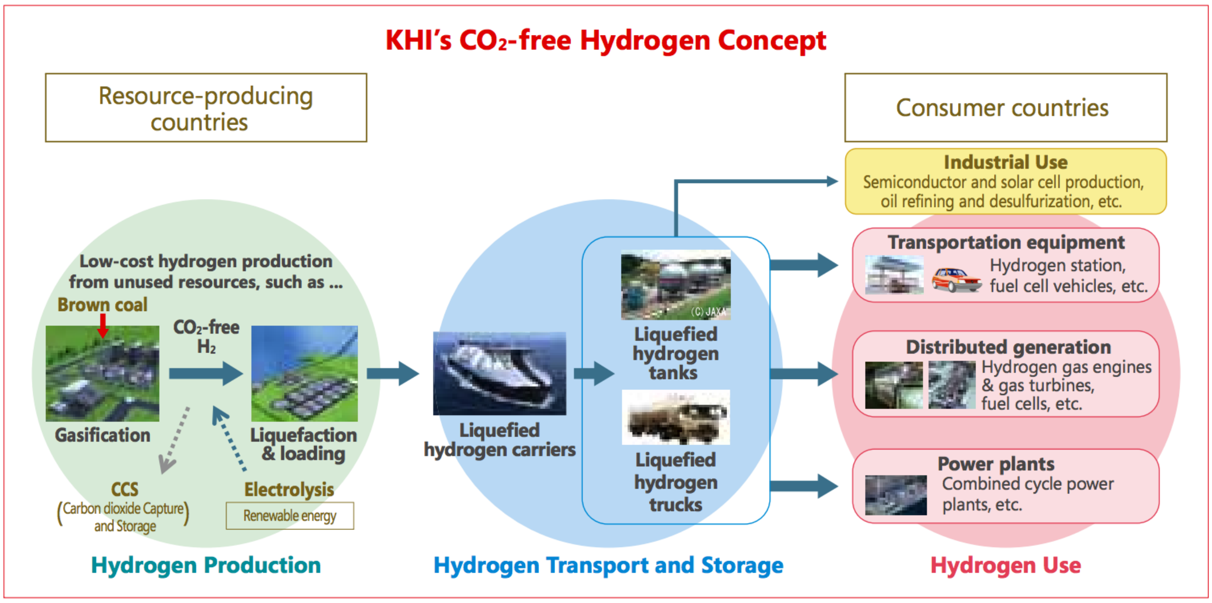

Figure 4. KHI's CO_2 free hydrogen concept.

The concept is currently going through the stage of basic engineering with a go / no go on pilot demonstration – 10^3 kg/day hydrogen plan – decision scheduled in March 2014. The pilot chain operation is planned for 2017 and if successful full demo chain operation to start by 2025. The full capacity is planned at $770 \cdot 10^3$ kg/day of liquid hydrogen. This amount would be enough to fuel 3 million Fuel Cell Electric Vehicles (FCEV) or run a Hydrogen Fuel Cell (HFC) power plant with 650 MW electric capacity.

Such a significant large-scale operation poses safety challenges related to storage and transportation of large quantities of hydrogen. For example, if hydrogen is in the liquid state the ground storage would require an overall volume of 250,000 m^3 with 5 vessels 50,000 m^3 each, while maritime transport will require 160,000 m^3 capacity per ship with 4 tank units 40,000 m^3 capacity installed on each of two ships.

The biggest knowledge gap here relates to appropriate / optimized safety distances as well as certain elements of safety design like a burn pond or a dike for secondary containment. Existing methods for calculation of safety distances for liquid hydrogen are based on data obtained in early 1960's - 1970's. Those correlations did not anticipate such significant amounts and as such cannot be used for reliable calculations. New engineering tools are needed.

A similar situation is with the shipment of large quantities of LH_2. Large bulk transportation is not covered by any code or standard.

In summary, more knowledge is required related to

- Spillage of large quantity of LH_2 on ground or seawater
- Cloud dispersion of cold hydrogen from vent and its ignition
- Performance of various thermal insulation options
- Safety distance as function of LH_2 quantity and re-assessment of the scientific basis for existing correlations
- Evaluation of related hazards and their consequences
- Risk assessment of typical accidents.

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2. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN DETERMINISTIC AND RISK-INFORMED SAFETY SCIENCE AND ENGINEERING

EXECUTIVE SUMMARY

The safe use of any technology and associated facilities requires that that the hazards and associated risk be understood and minimized. This can be accomplished by performing a hydrogen safety engineering (HSE) of a system or sub-system or an entire quantitative risk assessment (QRA) where hazards are identified, possible accident scenarios are delineated, acceptance criteria are formulated, and the resulting consequences are evaluated and used along with respective probabilities. QRA has been used to evaluate the risk associated with hydrogen facilities, for determining separation distances, and in land use planning. The results of these analysis have been successfully implemented in model code development. Although the general methods for performing a QRA are well established, there are significant gaps in the data needed to establish the frequency of accidents and in the deterministic models used to evaluate the resulting consequences. In addition, the current applications of QRA have been incomplete in that they have not addressed all hazards.

There are several benefits to performing a hazard and risk assessment, either qualitative or quantitative, for a hydrogen facility such as a fuelling station. The most important benefit is that it provides a systematic framework for identifying what can go wrong at a facility and what can be done to prevent or mitigate possible accident scenarios. Thus, the results from a hazard and risk assessment provides insights on ways to improve the safety (i.e., reduce the risk). The qualitative insights identify how to reduce the potential for accidents and the resulting consequences regardless of the risk significance of the accident but provide limited insights on which improvements will provide the greatest reduction in risk. Those types of insights are available from the quantitative results of a QRA which makes it a more powerful tool than qualitative methods such as failure modes and effects analysis (FMEA) for ensuring the safe design and operation of a facility, etc.

The results of a safety analysis can be used in a science-based, risk-informed process to establish requirements for the inherently safer design and operation of hydrogen systems and facilities. A science-based, risk-informed process utilizes science, engineering, and risk insights obtained from QRAs combined with other considerations to establish requirements. The QRAs are used to identify and quantify scenarios for the unintended release of hydrogen, identify the significant hazard and risk contributors at different types of hydrogen facilities, and to identify potential accident prevention and mitigation strategies to reduce the hazards and associated risks to acceptable levels. Examples of considerations used in this risk-informed process can include the results of science-based deterministic analyses of selected accidents scenarios, good hydrogen safety engineering (Saffers and Molkov, 2013) practices such as the inclusion of defence-in-depth for certain safety features (e.g., protection against pressure and thermal effects) and the use of safety margins in the design of high-pressure components, and requirements identified from the actual occurrences at hydrogen facilities when they are available. A key component of this process is that both accident prevention and mitigation features are included in the design and operational requirements.

STATE OF THE ART

QRA methodology

Hazards associated with a system or a facility are typically identified using a variety of qualitative techniques including FMEAs. Different types and levels of hazards are typically identified which can lead to accident scenarios. The accident scenarios can be delineated using tools such as fault and event trees which identify the hardware failures, human errors, and phenomenological events that lead to varying levels of undesired consequences to people, property, and environment. The frequency of the accident scenarios are evaluated utilizing a combination of failure data and conditional event probabilities (e.g., ignition probability). The consequences are evaluated utilizing a variety of deterministic tools that can range from simple engineering models to sophisticated computational fluid dynamics (CFD) analysis. In QRAs, models such as Probit functions are utilized to translate the adverse environments predicted by deterministic models into probabilities of harm to people or damage to components or structures. The frequency of identified accidents and resulting consequences are combined to evaluate the risk associated with the operation of a facility which contributes to the overall perception regarding the safety of hydrogen use (risk is a measure of safety (Tchouvelev, 2007); whereas safety is defined as freedom from unacceptable risk (ISO/IEC Guide 51). The type of information that is utilized in a QRA of a hydrogen system or facility is depicted in Figure 2.1.

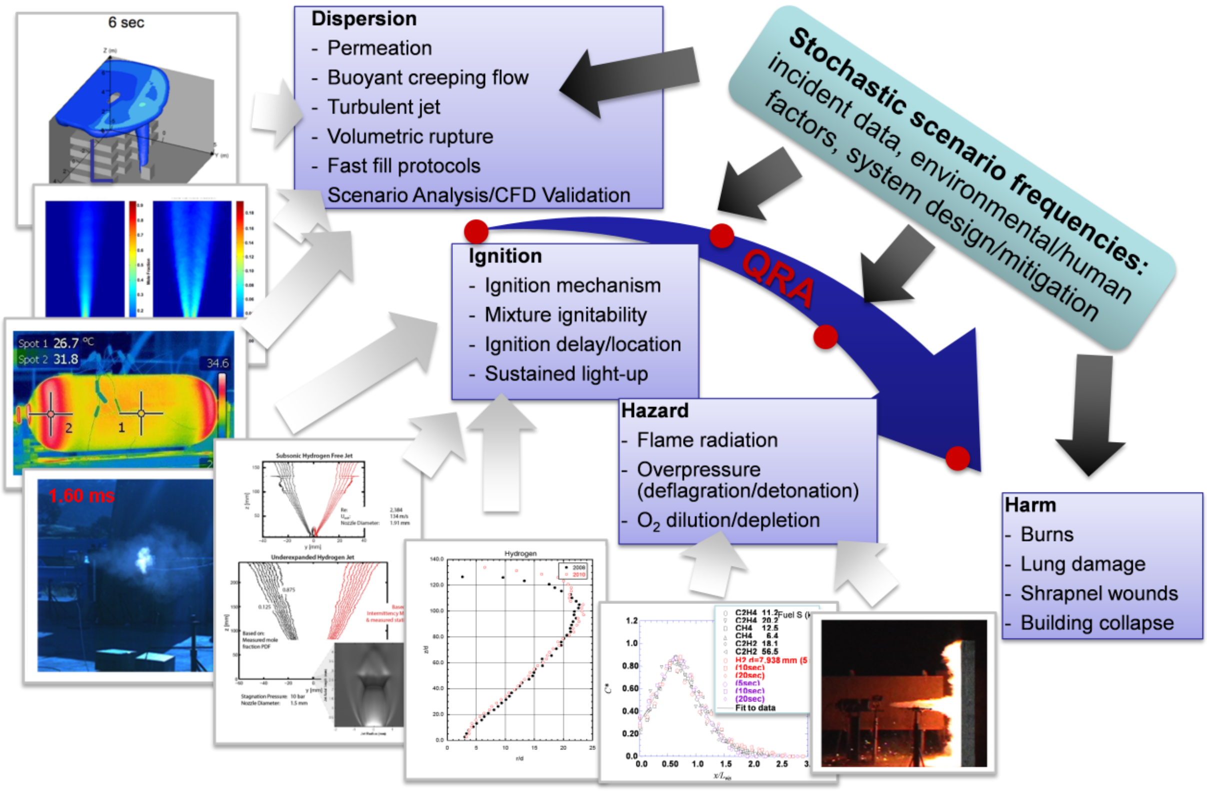

Figure 2.1. Information needed to quantify a QRA.

Hazard identification is the initial step in either hydrogen safety engineering or risk assessment. The purpose of the hazard identification is to identify all events that can affect facility operation leading to a hazard to individuals or property. It involves not only the identification of accident initiators but also considers the potential scenarios that lead to harm to individuals or property. The risk analysis can also include a rough order of magnitude assessment of the frequency and consequences of the identified scenarios which is generally used to rate the criticality or importance of individual scenarios. Fundamental methods such as Hazard Identification (HAZID), Hazard and Operability (HAZOP) studies, FMEA, and WHAT-IF analysis (AICE, 2000) are examples of tools which can be used to identify the hazards and assess the criticality of possible outcomes. These methods also have the advantage of being sufficiently general for use on hydrogen facilities without specific adaptation. A necessary feature of all these methods is that they should be performed by a multidisciplinary team that should include design and operations personnel with technical experience and expert knowledge of the facility design, owner and first responders, as well as someone who is independent and can take an objective view of the design, e.g. hydrogen safety engineer. In one of these processes, Rapid Risk Ranking (EIHP2, 2002), hazard identification is used as a screening process where events with low or trivial risks are dropped from further consideration. However, a major pitfall with this and similar approaches is that rough order of magnitude frequency and consequence evaluations are used to evaluate and screen scenarios. Since screening is done at a scenario level, the risk associated with all of the screened scenarios could be significant leading to an under estimation of risk. In case of significant probability of catastrophic failure among all possible failures, e.g. at level of 10% of total failures, a risk should be assessed based of consequences of a catastrophic failure of a system or facility element(s). Guidance on the proper use of these semi-quantitative hazard identification methods as screening tools and associated screening criteria is required.

In a QRA the total risk is calculated by taking the sum of the risk associated with each identified accident scenarios. In most QRAs of hydrogen facilities performed to date, the different potential accident scenarios have been delineated in event trees. Event tree analysis systematically explores the potential accident scenarios that can occur following an accident initiating event which is influenced by accident phenomena, mitigation system response, and operator actions. The event tree displays the sequences of events involving success and/or failure of the system components, and results in the identification of accident scenarios including their consequences and frequencies. The failure modes of mitigation systems can be depicted in fault trees. The accident scenario probabilities (frequencies) and consequences establish the individual scenario risk which can be summed to provide the overall facility risk (see LaChance, et al., 2009 as an example of this approach). The integration of the risk in a QRA requires for the identification of the initiating events, accident scenarios, human errors, and component failures that contribute the most to the facility risk. An alternative, well known approach to accident sequence evaluation using Bayesian Belief Networks (Fenton and Neil, 2013) has been utilized by in hydrogen applications (Haugom, et al., 2009, and Pasman and Rodgers, 2011).

In order to quantify the accident sequence models, data for the modelled events must be obtained. The required data includes the frequency of accident initiating events (e.g., hydrogen leaks), component failure probabilities, human error events, and the probability of certain accident phenomena. The initiating event frequencies and component failure and human error probabilities required in a QRA can be obtained directly from historical records where available. Similarly, conditional event probabilities can be estimated for inclusion in accident sequence models such as event and fault trees. For example, historical information can be used to estimate the conditional probability of auto-ignition of a hydrogen jet following a release A detailed discussion of the data analysis process, including common statistical methods, is provided in Atwood et al., 2003. Unfortunately, there are little hydrogen-specific data available, no requirements for collecting data (the exception being the U.S. Department of Energy's (DOE) technology validation (Spirik, et al., 2011), and current data collection efforts such as in the IA HySafe *Hydrogen Incident and Accident Database* (JRC, 3013) and the U.S. DOE's *Hydrogen Incident Reporting and Lessons Learned* database (PNNL, 2013) are not sufficient for utilization in a QRA. Thus, data from other industries, primarily the oil and gas industry (e.g., HSE, 2001) has been utilized in hydrogen facility QRAs. A different approach using a Bayesian process to combine limited hydrogen data with data from other industries was used in LaChance, et al., 2009. Without hydrogen-specific data, the fidelity of hydrogen QRAs is less than desirable contributing to the uncertainty in the resulting risk estimates. Thus, currently the deterministic hydrogen safety engineering methods prevail over the probabilistic methods for a design of particular system or facility. At the same time probabilistic risk-informed methods were successfully applied to demonstrate that hydrogen technologies are not more risky compared to current fossil fuel technologies (LaChance, et al., 2009).

In any application, humans can make errors resulting in dangerous situations that initiate or contribute to accidents. In fact human errors are often significant contributors to accidents. In general, human errors occur as a result of the lack of familiarity or experience to perform a required task or because they make a slip or error in performing required actions. Human errors resulting in accident initiating events can be identified as part of the hazard identification process discussed previously. Human errors that can exacerbate an accident sequence are identified as part of the event and fault tree construction process. The process of quantifying these human errors is referred to as human reliability analysis (HRA). There are many HRA methods that can be utilized to quantify the identified human errors. Each has their own strengths and weaknesses and some are more appropriate than others for specific applications. A description of many of these methods is provided in Forester et al., 2006 along with an evaluation of their capability to satisfy accepted good practices (considering the current state-of-the-art) for performing an HRA (Castiglia and Giardina, 2013 has recently compared two HRA methods as applied to quantifying maintenance errors in a refuelling station). To date, human errors have not been generally explicitly included in hydrogen facility QRAs (one recent exception is in Groth, et al. 2012). This lack of explicit treatment especially in light of the lack of hydrogen–specific accident data may result in a significant under prediction of the risk of operating a hydrogen facility.

A key parameter in the evaluation of hydrogen accident scenarios is the probability of ignition. The resulting consequences of a hydrogen release are dependent upon whether the hydrogen is ignited immediately (e.g., due to the effects of the release) or is delayed (e.g., due to an external ignition source). There has been much work on the potential for self-ignition and delayed ignition of hydrogen jets (see Chapter 5) but to date it has not been translated into a probabilistic model that is needed in QRA due to lack of deterministic knowledge specific for hydrogen. However, efforts have been made to develop ignition probability models based on literature searches, empirical data, and some experimental data. A review of existing hydrogen ignition probabilities and data from hydrogen incident databases was performed in the HySafe project (Rodsaetre and Holmefjord, 2007) and utilized to generate a suggested hydrogen self-ignition model based on an existing hydrocarbon model. However, ignition probabilities from many sources including the Purple Book CPR18E, 1999) have been utilized in hydrogen facility QRAs. Unfortunately, uncertainties of these probabilities are not clear. LaChance, et al., (2009) utilized hydrocarbon ignition probabilities modified by Tchouvelev, (2006) to account for hydrogen properties and performed sensitivity studies indicating that the uncertainty in ignition probabilities was the major contributor to the uncertainty in the overall risk results along with uncertainties in consequences of initially unignited releases (e.g. an extent of a flammable envelop, as in case of an attached jet, or an overpressure of a delayed ignition deflagration, which is still a serious knowledge gap), and ignited releases (outdoors and indoors jet fires). Thus, more work in establishing a probabilistic ignition model based on hydrogen-specific deterministic experimental, numerical and analytical information is required to obtain acceptable fidelity risk assessment results.

Event tree analysis results in the development of the different accident scenarios including the end states of those scenarios. Consequence calculations are generally performed for each of the identified end states and combined with the scenario probability (frequency) to determine the risk associated with the scenario and identified hazard(s). The consequence calculations should predict the physical circumstances resulting specifically from the accident (e.g., pressure effects of hydrogen releases, fires and deflagrations/detonations, as well as thermal radiation levels, etc.). The consequences are usually quantified using models; these may be either simple engineering tools or contemporary Computational Fluid Dynamics (CFD) models. The state of the art in the deterministic analysis of hydrogen behaviour and consequences is discussed in Chapters 3, 4, 6, and 7 of this report. Engineering tools are usually based on a simplified representation of the physics of underlying phenomena obtained by analytical models or semi-empirical and empirical correlations of experimental data. Because they are based on the simplified models and correlation of limited experimental data, engineering tools can have a limited range of applicability and caution must be exercised so as to not extrapolate the results of the model beyond the applicability range. The simplified engineering models are generally conservative but are relatively easy to use and are fast running. CFD modelling and simulations involve solving of a set of governing partial differential equations which in most cases are conservation of mass, momentum, energy, and species mass fractions and turbulence quantities which are strongly coupled and highly non-linear in nature. CFD simulations can take long time and thus are not always practical for QRAs where the consequences from a large number of scenarios may have to be evaluated (unless scenarios are "blocked" in major groups without an increase of risk assessment uncertainties). Thus, there is a need to develop more reliable and validated simple engineering models for use in hydrogen safety engineering and QRAs. This need is addressed further in Chapter 8 of this report.

The results of consequence evaluations must be translated into a probability of causing damage to life, property and environment for use in a QRA. This can be done using Probit functions which provide a statistical correlation between the magnitude of the consequence (e.g., thermal heat flux) and the resulting potential for damage. A good summary of Probit functions is provided in LaChance, et al., (2011) and included Probits proposed in TNO, 1989 and used in some hydrogen facility QRAs. A major limitation of available thermal heat flux Probits (see for example Eisenberg, et al., (1975) and Tsao and Perry (1979)) is that they are not hydrogen-specific and thus lead to an area of uncertainty in the risk results (Probits for overpressure effects are independent of the source of the overpressure, e.g. deflagration/detonation or a blast wave from a ruptured storage tank, and thus can be utilized for hydrogen applications). Thus, development of a hydrogen-specific Probit function to estimate the probability of thermal heat flux damage is desirable to remove uncertainty in the QRA results (alternatively, sensitivity studies can be performed as recommended in LaChance, et al. (2011)).

In order to utilize the results of a QRA to make a risk-informed decision, it is necessary to establish risk acceptance criteria. There are different types of risk criteria including those for individuals (separate criteria may be specified for workers and users of the facility and for people located near the facility) and for the population surrounding the facility. A good summary of potential risk measures is provided in Jonkman, et al., (2003). Each country has its own risk criteria. Some countries utilize the As Low As Reasonably Practicable (ALARP) principle which specifies an intolerable risk level that must met regardless of cost and a tolerable risk level below which no action is required to reduce the risk. In between these regions, risk should be reduced if it can be accomplished in a cost-beneficial manner. Suggested uniform risk acceptance criteria for use in the hydrogen industry utilizing the ALARP principle were presented at the 2008 World Hydrogen Energy Conference (Tchouvelev, et al., 2008) based on a survey of types and values of risk criteria in general use. A suggested cost-benefit criterion for utilizing the ALARP principle on hydrogen facilities was not included in the recommendations.

Finally, when documenting the results and conclusions of a risk assessment it is necessary to address the robustness of the results taking into account the uncertainties in the analysis. Uncertainties in hydrogen system or facility risk assessment result from many sources including: sparse data on hydrogen accidents, lack of understanding on phenomena (e.g., ignition, fire, deflagration/detonation, high pressure hydrogen storage tank rupture in fire conditions, etc.), modelling assumptions (e.g., leaks modelled as circular orifices instead of leak through cracks that is rather plane jet), modelling limitations (e.g., inability to model surface effects for attached unignited jets and jet fires), and incompleteness (lack of analysis of external hazards such as earthquakes and high winds). To appropriately account for the uncertainties in the QRA results in decision making, a thorough understanding of deterministic phenomena, the reliable probabilities of events for the QRA model are required. This understanding will identify the underlying assumptions and limitations, thereby indicating the sources of uncertainty in the QRA results and insights. Understanding the sources of uncertainties will indicate the parts of the QRA model that could be affected (practically all at the moment), and ultimately the results from the QRA model that will be impacted. Guidance on making decisions in light of uncertainties is needed and can potentially be adapted from other industries (e.g., see NRC 2013). The assessment of uncertainties level is of paramount importance in QRA as it is clear that if uncertainties level is comparable with an acceptable risk level then results of QRA are hardly acceptable for practical purposes.

Application of QRA

The insights from a QRA can be used in several areas. First, the results can be used in a generic fashion to risk-inform regulations, codes, and standards (RCSs). The minimum design and operation features necessary to ensure an acceptable level of risk to the public (with taking into account uncertainties), workers, and users of a facility can be established in a QRA and subsequently prescribed in RCSs requirements. Since in many countries authorities having jurisdiction (AHJ) rely on compliance with well-known codes and standards as one means to license a facility, establishment of risk-informed performance-based codes and standards is critical to ensuring the safety of these facilities along with development of contemporary methods for hydrogen safety engineering. An example of the use of QRA to establish code and standard requirements in USA is the generation of risk-informed separation distances in the NFPA 55 standard (LaChance, et al., 2009).

Although separation distances are a key safety parameter specified in hydrogen codes and standards, there are other design and operational requirements that are used to ensure safe operation. Key design features currently specified in hydrogen codes and standards include interlocked leak detection and isolation capability, dilution ventilation, emergency venting, emergency manual shutoff switches, pressure relief devices and associated vent lines, process monitoring and safety interlocks, and fail safe design requirements (e.g., closure of isolation valves on loss of power). Compliance with RCS requirements to separation distances has to be demonstrated rather than taken as granted. Indeed, there are examples when piping of internal diameter of about 20 mm from storage of 700 bar to dispenser is used (far above the technological needs for mass flow rate) with separation distance below 10 m (only flame from such pipe would reach more than 50 m). Operational requirements can include normal operating procedures, maintenance and surveillance procedures, limiting conditions of operation, and emergency procedures in the case of major accidents. Work to risk-inform hydrogen code and standard requirements pertaining to some of these features has occurred and is in progress at the National Fire Protection Association (USA) through the efforts of Sandia National Laboratories (see for example LaChance 2011 and Groth, et al., 2012).

In some countries, in addition to meeting code and standard requirements, regulations require a QRA be performed for hydrogen facilities and that the facility meet risk acceptance guidelines or criteria. There are examples of this type of application in the literature including those documented in Maththijsen and Kooi, (2006), Kikukawa, et al. (2009), and Zhiyong, et al., (2010). The development and application of QRA in regulatory efforts will likely increase as the use of hydrogen increases. In fact, a comprehensive risk analysis of major portions of the hydrogen infrastructure has been performed and is summarized in Rosyid (2006).

Finally, the results of QRAs will identify important hazards (e.g., random component failures or external hazards such as vehicle crashes, high winds, or earthquakes), accident sequences (typically hydrogen releases with ignition leading to fires or explosions), and consequences (e.g., thermal and pressure effects on people and equipment/structures). A full scope QRA would include a comprehensive evaluation of a range of potential accidents and thus is a useful tool to help prioritize research resources on both the significant contributors to risk and on where there are large uncertainties in the risk results. However, the full probabilistic QRA is a very expensive exercise and often can be substituted by deterministic or probabilistic studies of parts of the system or infrastructure. The results of QRAs are thus useful for identifying important gaps in our knowledge of hydrogen behaviour, including the information depicted in Figure 1 needed to quantify a QRA. Specifically, QRA results can identify the data needed to evaluate the frequency of accidental releases of hydrogen and can also help prioritize research for evaluating the behaviour and dispersion of hydrogen (see Chapters 3 and 4), potential for ignition (see Chapter

5), and subsequent behaviour during combustion (see Chapters 6 and 7). Use of QRA to prioritize hydrogen research has not yet been attempted.

IDENTIFICATION OF KNOWLEDGE GAPS

Although the current knowledge on hydrogen behaviour is well established, there are still numerous gaps in knowledge that would be needed to perform high quality hydrogen safety engineering and QRAs for use in risk-informed decision making. There are knowledge gaps in the evaluation of the progression of accident scenarios that leads to consequences, and especially their frequencies that undermines the quality of risk assessment methods. In addition, guidance is needed to address the application of QRA in risk-informed decision making including the consideration of uncertainties. The following gaps have been identified in the preceding discussions as well as in Pasman (2011), and Groth, et al., (2012).

- A defensible probability model for hydrogen ignition originating from recent deterministic studies, in particular on so-called "diffusion ignition". Current ignition probability models greatly oversimplify the variety of complicated ignition processes, and lack an underlying scientific basis for their use.

- Probability models for gas and flame detection, and other indoor-only components. There is not sufficient information on the accuracy of flame and gas detection in the hydrogen industry.

- Simplified models for predicting accident consequences, specifically the loads from deflagration and detonation for different release sizes. Due to the complexity of CFD codes, it is not possible to perform a complete CFD analysis for every possible accident scenario.

- Hydrogen-specific data for use in QRA evaluations. Current data collection efforts in the hydrogen fuelling industry are not designed to provide the detailed information necessary for use in QRAs. It is important to begin planning and testing an industry-wide framework for QRA data collection activities.

- Consideration of human, software, and organizational failure drivers. Hydrogen accident models and accident scenarios must be expanded to include plausible human failures, software failures, and organizational failures that can result in hydrogen releases.

- Guidance and criteria for the screening and evaluation of external factors from risk assessments. External factors such as high winds and earthquakes may be significant risk contributors. A pilot study of these hazards would be beneficial.

- Development of hydrogen-specific harm criteria (specifically a Probit function) for thermal heat flux. Existing harm criteria do not reflect the thermal spectrum emitted by hydrogen flames.

- Guidance on the use of risk insights in decision making. The scope of the risk assessment, the value of the estimated risk compared to risk criteria, and consideration of uncertainties in data and models should all be considered when making risk-informed decisions.

- Uniform cost-benefit criteria for use in evaluating acceptable risk levels. This is needed to determine how many accident prevention and mitigation features should be required and for determining which features are most cost effective.

In addition to the above gaps, there is a need for further applications of QRA to address the risk in the hydrogen infrastructure including vehicles. Development of a QRA toolkit would facilitate the application of QRA to risk-inform RCS and design and operate hydrogen facilities (i.e., help specify risk management capabilities). Such a toolkit would include validated models and data specific for hydrogen applications and thus would enhance the quality of hydrogen facility. In addition, the presence of simple validated phenomenological models (see Chapter 8) in such a toolkit would greatly facilitate the performance of a QRA as well as the deterministic evaluation of accident scenarios.

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3. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN SOURCE, RELEASE AND DISPERSION FOR GASEOUS H2

EXECUTIVE SUMMARY

The evaluation of the safety of hydrogen systems and infrastructure requires methods to characterize the release of hydrogen and the determination of the extents of the flammable clouds and hot gas flow produced by hydrogen jet fire, which are very important parameters in the establishment of the safety (separation) distances and sizes of hazardous zones. Jets and plumes are the most common types of hydrogen releases. As such, their properties have been studied extensively by hydrogen safety researchers. The scaling behaviour of the concentration field in the expanded region of jet releases have been characterized analytically, studied numerically and validated experimentally. The effect of buoyancy on the concentration profile along the centreline of the jets has been examined using integral models, assuming a transverse Gaussian distribution of hydrogen in air. A comparative study of the relative validity and limitations of notional nozzle approximations has been performed, using various turbulence modelling strategies and experimental data. Notional nozzle approximations are generally introduced to reduce the level of modelling details and of grid refinement required to properly describe the shock wave structures generated close to the nozzle by sonic and super-sonic releases. These studies have ranked 5 commonly used models for hydrogen jet releases in terms of predictive capacities. Further studies would evaluate their predictive capabilities as a function of flow properties. More detailed comparison involving the effect of notional nozzle approximations on the spreading of the release and the effect of obstacles close to the notional nozzles are still needed. Preliminary work on the effect of proximity of surfaces along jets has been performed, showing an increase of the flammable length of jet releases with potential consequences on hazard analysis, and interesting effects on the scaling properties of jets. Experimental validation of these studies is still required along with analytical theories for scaling of attached jets and fires. Much numerical and analytical work has also been done on slow and fast releases of hydrogen in enclosures (such as garages). Computational fluid dynamics (CFD) simulations have been extensively used to study hydrogen releases and their dispersion, bringing the issue of the validity of various approximations and models used to perform those simulations to the forefront of hydrogen safety research and engineering. In this context, benchmarking and model/tools validation exercises, originally initiated by the European Network of Excellence HySafe (NoE HySafe), are still being pursued in the context of the International Association for Hydrogen Safety (IA HySafe) to explore the usefulness and limitations of the modelling strategies and numerical approximations commonly used in CFD simulations. These exercises should lead to the instigation of a standard validation matrix for CFD simulations that could be used as benchmarks for dispersion simulations as well as for simulation of other phenomena relevant to hydrogen safety.

STATE OF THE ART

Properties of jet releases

Jet releases have been the object of intense R&D activities. An overview of the properties of neutrally buoyant turbulent jets (compressible and incompressible) is presented in the classic work of Abramovich, et al (1963). The scaling properties of momentum-controlled vertical turbulent jets are detailed in a monograph by Chen and Rodi (1980). The rate of decay of the concentration field as a function of distance jets and plumes (laminar and fully turbulent) are summarized in Table 1 of their work. Expansion of the similarity law by Chen and Rodi (1980) to under-expanded jets and its validation for both expanded and under-expanded jets is described in Molkov (2012).

Scaling properties of the concentration field and the effect of the shape of the release

For turbulent jets, it was shown that the concentration field decays as the inverse of the distance to the source for round jets and the inverse of a square root of the distance for expanded (!) planar jets. Jets from non-circular orifices with aspect ratios far from unity are expected to exhibit the behaviour of planar jet with an eventual crossover to the behaviour of round jets far from the source. Near field studies of jets originating from elliptic orifices of various aspect ratios have been performed extensively in the past, for instance in the context of jet acoustics (Verma, et al., 2001), and recently by Paraschivoiu, et al in the context of self-ignition of hydrogen jets (Shishehgaran, et al., 2013). The study of hydrogen decay in highly under-expanded jets has been published recently by Makarov, and Molkov (2013). Detailed studies on the effect of the shape of the orifice on the concentration field of hydrogen in the expanded region seem, however, to be far from completion, despite the fact that realistic sources are likely to be linear and even annular.

Notional nozzle approximations

In 1984, Birch et al proposed, in the context of gaseous hydrocarbon fuels, a methodology to evaluate the decay of the mean concentration field along the centreline of a supercritical free jet using their notional nozzle approach (Birch, et al., 1984). Unfortunately, the similarity law in the form developed by Chen, and Rodi was published with three major differences as described by Molkov (2012). The distance taken for the mean mass fraction concentration to decay to a given value in such flows is proportional to the diameter of the source and inversely proportional to the square root of the density of the jet fluid in the nozzle (Molkov 2012). Birch, et al. (1987) later reformulated their effective diameter definition based on the conservation of both mass and momentum. Houf, et al (2005) used the Birch approach to determine the concentration decay of under-expanded hydrogen jets taking for the first time into account non-ideal behaviour of gas at high pressures. In their implementation, they reformulated the effective diameter of the pseudo-source by replacing the velocity at the end of the expansion region by an effective velocity, as originally suggested by Hess, et al (1973) for under-expanded gas jets. They also removed the discharge coefficient in the effective diameter definition. The original theory to calculate concentration decay in under-expanded hydrogen jets without using notional nozzle diameter but density of hydrogen at real nozzle exit instead was developed and successfully validated at Ulster by Molkov, et al. (2012). This novel approach demonstrated that the similarity law in the original form suggested by Chen and Rodi can be applied to both expanded and under-expanded jets without modification.

Described above approaches have been extensively used to eliminate the need of carefully considering the shockwave structure of sonic jets close to the nozzle in order to reduce computational requirements for numerical simulations when applicable, e.g. for free jets.

The jet is assumed to originate from a pseudo-source (the notional nozzle) with an effective diameter and effective uniform boundary conditions (temperature, jet velocity). This effective source does not have a direct physical significance. Its properties depend on several approximations on the governing equations, and generally assume uniform properties (velocity, concentration, temperature) at the effective inlet. Several strategies have been proposed to derive the properties of the notional nozzle. They can be classified according to the conservation equations considered, and to the assumptions made for the temperature of the gas at the notional nozzle. Typical modelling strategies are based on a three stage lumped parameter approximation (inside the storage unit, at the actual orifice, at the effective nozzle exit). Other approaches rely on the properties of the Mach disk, such as the jet models developed by Winters, et al (2007) and by Gexcon for their FLACS solver (2008). In addition to the conservation equations, both use the normal shock relations to specify the flow properties at the various stages. The Winters approach assumes isentropic flow in the expansion between the orifice and the Mach disk, and uses the Abel-Noble equation of state (EOS). The Gexcon jet model assumes adiabatic expansion and relies on the ideal gas EOS. The models yield an effective orifice through which the full flow is assumed to originate. Such approaches assume that all the gas passes through this effective Mach disk, which constitute an unverified approximation. Both approaches yield similar predictions. Dispersion simulations performed with FLACS using this notional approximation yields, however, results consistent with experiments over broad ranges of conditions (Baraldi, et al., 2009; Venetsanos, et al., 2009).

A detailed evaluation of recent notional nozzle models for free-shear under-expanded hydrogen jets has recently been performed by Papanikolaou, et al (2012). They compared five notional nozzles (references), based on various assumptions as described in Table 3.1 below.

Table 3.1. Comparison of notional nozzle approximation models (Papanikolaou, et al [11])

Model	Conservation equations			Equation of state	Temperature (T) at the notional nozzle
	Mass	Momentum	Energy		
Birch 1984	X			Ideal gas law	Ambient
Birch 1987	X	X		Ideal gas law	Ambient
Ewan[12] 1984	X			Ideal gas law	Actual nozzle
Schefer [13] 2007	X	X		Abel-Noble	Ambient
Harstad [14] 2006	X	X	X	Ideal gas law	Immediately after Mach disk

Simulations were performed for each model using three turbulence models (the standard k-ε model, the baseline k-ω model and the shear-stress transport approach) and compared with experimental data for jet releases from three orifice diameters (0.25, 0.5 and 1 mm) performed at the Karlsruhe Institute of Technology. Given a turbulence modelling strategy, the best accuracy was obtained when using the notional nozzle approximation of Birch, et al (1987) and Schefer, et al (2007), followed by Birch (1984) and Ewan, et al (1984), and finally Hastard (2006).

Although recent studies confirm that the far-field features of an under-expanded jet release can be successfully modelled using notional nozzle approximations with various degrees of success, important issues remain to be addressed. It remains unclear to what degree such approaches can be applied to the description of attached or confined jets, particularly when the source is located in close proximity to a surface. A detailed analysis of the effect of this approximation on the transverse velocity distribution of under-expanded turbulent jets as a function of position along the axis of the jet should also be performed. The applicability of notional approximations to different shapes of the orifice of the release has not yet been looked into in details and seems hardly applicable for characterisation of concentration decay in plane jets that needs further investigation.

Buoyant jet releases

The scaling behaviour discussed in the preceding sections is based on the assumption that the jet is fully developed and momentum-driven throughout its volume. For realistic jet releases, the development of the boundary layer of jet releases is indeed initially driven by the momentum of the injected gas. However, because of the low density of hydrogen, buoyant forces eventually affect the behaviour of the jet. Far enough from the origin, the jet becomes increasingly affected by buoyancy. The driving force for the development of the boundary layer of the release eventually becomes the buoyant force. This region of the jet is defined as the plume region. The importance of buoyant forces can be quantified by the Froude number, which is a measure of the relative importance of gravity and momentum forces. Different forms of Froude number are applied to characterise transition from momentum- to buoyancy-controlled flow in the release (Molkov 2012). For example, the densimetric Froude number is defined as follows:

$$Fr_{den} = \frac{U_{exit}}{\left(\frac{gD(\rho_{\infty}-\rho_{exit})}{\rho_{exit}}\right)^{1/2}}. \quad (1)$$

Buoyant jet releases occur for small scale, often subsonic releases. Such releases do not in principle follow the scaling laws for momentum-controlled jets described earlier. Buoyancy-controlled releases decay faster than momentum-dominated. Thus, the similarity law for momentum-controlled jets can be used as a conservative estimate for any jet. Buoyant jet (plume) behaviour can however be predicted numerically if required. Low momentum hydrogen jets (forced plumes) have been studied by Houf and Schefer (2008). They measured the mass fraction of low momentum vertical jets (Froude numbers of 99, 152, 268) and compared the results with an integral model they proposed, based on momentum and mass balance, and an entrainment coefficient that takes into account momentum (Ricou, et al., 1961) and buoyancy (Hirst 1971) contributions. A non-Boussinesq engineering model was proposed by Xiao, et al (2009) for fully turbulent horizontal jets. Their model also assumed a scaling behaviour normal to the axis of the jet, included the energy equation and took into account large density variations in the entrainment coefficient. They obtained good agreement with experimental data (with small density variations) and CFD simulations (with large density variations) performed with GasFlow. They noted that the Boussinesq approximation was only valid if the density variations were less than 10%.

Deviations from the scaling behaviour of expanded jets along the centreline of the jet for subsonic low momentum horizontal jets (which could be defined operationally as the curve representing the positions of the local maxima of the concentration profile of the jet) are discussed in reference (Hourri 2011).

Predicting the scaling behaviour of the concentration as a function of distance is useful for hazard analysis as it allows for the definition of exclusion zones based on the lower flammability limit of hydrogen. It is interesting to note that Molkov and Saffers recently (Molkov, et al., 2011) established a general correlation for the length of hydrogen flames normalized by the nozzle diameter as a function of the product of the ratio of the density of hydrogen at the nozzle to the ambient density of the environment by the cubic power of the Mach number. This correlation was shown to be applicable to all three flow regimes, including both buoyancy and momentum-dominated (the last is subdivided into two – for expanded and under-expanded jets). In view of the fact that there are indications that the flame length may be correlated to the size of an unignited jet where concentration is 11% by volume in average (changes from 8% to 16% for the range of experimental data investigated) (Molkov, et al., 2012), it would be interesting if a corresponding correlation could be derived for the flammable envelope size of a hydrogen release.

Behaviour of jets close to surfaces (attached jets)

The proximity of jets to surfaces will modify the scaling behaviour of expanded jet and typically increase their flammable lengths, which can be defined as the distance from the nozzle to the point where the concentration field drops to the lower flammability limit (4% by volume for hydrogen). Proximity effects on jet releases can play an important role when performing hazards and associated risk assessments (for instance in determining the consequences of a flash fire event, for which is usually assumed 100% lethal within the confines of the LFL). Proximity to a surface will modify the flow properties of the release. It may induce a Coanda effect, create a recirculation zone between the nozzle and the surface, and generate transient behaviour such as puffing, which may temporarily increase the flammable extent beyond the steady state equilibrium concentration profile for a short while after the release is initiated (Bénard, et al., 2007). The properties of attached jets have been studied numerically (Hourri, et al. 2010; Hourri, et al., 2008) and to a lesser extent experimentally for unignited (Désilets, et al., 2009) and ignited (Willoughby, et al., 2009) releases. Simulations using FLACS have been performed to examine the overall behaviour of hydrogen and methane jets over wide ranges of storage pressures (10-70 MPa). An interesting behaviour was observed for the normalized overextent of the flammable distance from the nozzle induced by the presence of the surface when expressed as a function of a normalized distance of the orifice from the surface. Because of the simple modelling assumptions that were used to enable the study of the wide range of conditions and the number of distances of the orifice to the surface, these results require experimental confirmation and cross-checking with simulation results obtained using more complex turbulence modelling. No analytical results and engineering tools are available for this important for safety design phenomenon.

Releases in enclosed areas

Hydrogen concentration build-up inside enclosed areas presents particular issues with respect to safety because of the reduced rate of dispersion and the increased chance that an ignition event leads to an explosion. The project InsHyde within the framework of the European NoE HySafe (Jordan, et al., 2011) has investigated realistic small-medium indoor hydrogen leaks and provided some recommendations for the safe use/storage of indoor hydrogen systems (Venetsanos, et al., 2011). Numerical and experimental studies show that hydrogen accumulation leads either to a stable, stratified distribution of concentration or to the formation of a homogeneous layer if the convective flows at the top of the enclosure are high enough (Cariteau, et al., 2011; Cariteau, et al., 2011; Zhang, et al., 2010). Simplified mathematical models have been devised to predict the dispersion of hydrogen releases within a confined volume (Benteboula, et al., 2009). The simple "natural ventilation" model predictions are in acceptable agreement with experiments for relatively long time gas discharges for jet like or plume like releases if the discharge coefficient is "turned" appropriately. Experiments on the mechanisms and kinetics of hydrogen-air flammable gas cloud formation and evolution due to hydrogen leaks below less than 10^{-3} kg/sec into confined spaces with different shapes, sizes have been conducted (Denisenko, et al., 2009). The experiments have shown two qualitatively different gas-dynamic patterns of flammable gas cloud formation and evolution termed as «filling box» and «fading up box». The occurrence of these patterns depends essentially on the speed of the hydrogen/helium gaseous release into closed space at constant flow rate. In a «filling box» case (at a low speed of hydrogen outflow), the flammable cloud initially forms as a thin layer at the ceiling and then expands via concentration front downward. In a «fading up box» case (at a high speed of hydrogen outflow), the flammable cloud forms nearly uniformly throughout the whole volume above the discharge point.

A study investigating the discharge of hydrogen from onboard storage tanks through a PRD inside a garage like enclosures with low natural ventilation has been performed (Brennan, et al., 2011). The goal was to investigate the relationship between PRD diameter, natural ventilation i.e. ACH: Air Change per Hour, and volume for releases in enclosures with a single vent from onboard storage tanks of 1, 5 and 13 kg at storage pressure 35 and 70 MPa. In an earlier work (Brennan, et al., 2011), the same authors investigated a hypothetical scenario, with a constant mass flow rate release where the "pressure-peaking phenomenon" following the unignited release of hydrogen through a "typical" PRD (diameter 5.08 mm) in an enclosure with a small vent was explained.

It was demonstrated, that for a constant release of 0.39 kg/s of hydrogen (unignited) into a 30.4 m^3 garage with a single vent the standard size of one brick the overpressure within the enclosure within 2 s, reaches a level of 10-20 kPa, which is capable of destroying the garage. A phenomenological model has been developed, and compared with CFD simulations to predict the pressure dynamics within an enclosure.

Computational fluid dynamics simulations

Computational fluid dynamics (CFD) simulations of hydrogen releases and their subsequent dispersions have the potential to be powerful tools to help assess the consequences of hydrogen releases, and to help study physical phenomena efficiently and to a high level of details. As such, a substantial body of work relying on CFD simulations have been generated, using diverse modelling strategies and various degrees of approximations, for problems representing widely ranging conditions. Issues such as the applicability and reliability of turbulence models, the proper treatment of boundary conditions, the validity of notional nozzle approximations, the proper treatment of surface effects, and grid sensitivity analysis constitute ongoing topics of discussions in the community. Benchmarking and validation exercises (*Standard Benchmark Exercise Problems or SBEP*), originally initiated by the European Network of Excellence HySafe (Venetsanos, et al., 2009), are still being pursued in the context of the international association (IA HySafe) to explore those issues and should eventually be the topic of a detailed, specific report. These exercises should lead to the instigation of a *standard validation matrix* for CFD simulations that could be used as benchmarks for dispersion simulations. The validation matrix would be constituted of state-of-the-art, high quality experimental datasets covering regions of parameter space applicable to hydrogen safety problems. A list of recent experimental datasets is presented at the end of *References* section.

Fast filling simulations

During the filling process of hydrogen tanks, the gas temperatures inside the tank can reach high values, potentially jeopardizing the structural integrity of the storage system and reducing the state of charge of the tank. Several research teams have performed CFD validation studies (Dicken, et al., 2007; Kim, et al., 2010; Zhao, et al., 2010; Heitsch, et al., 2011; Takagi, et al., 2011). By comparing the simulation results with the experimental data they demonstrated that the current CFD models are capable of capturing the maximum temperature histories inside the tank with a sufficient level of accuracy. CFD can be instrumental in identifying the best filling protocols for the RCS.

IDENTIFICATION OF KNOWLEDGE GAPS

The following issues are still considered as open from the perspective of the modelling of hydrogen release and dispersion for safety analysis.

- Effects of surfaces on jets (attached jets, impinging jets)
- Detailed validation of notional nozzle theories (proximity to a surface, effects of buoyancy, effects on the lateral concentration distribution, nozzles with small diameters) and other approaches allowing to eliminate simulation of shock structure of under-expanded jets
- Effects of the shape of a nozzle on the release (slits, elliptic orifices, rectangular orifices, effects of the aspect ratio of asymmetric orifices on the scaling laws)
- Constitution of a validation matrix for CFD simulations
- High pressure releases in enclosed areas (with passive or forced ventilation)
- Effect of wind on unignited jets
- Interaction of multiple jets
- Behaviour of jets from flapping sources
- Universal scaling law for the flammable extent of jets

- Behaviour and dispersion of cryogenic jets outdoors and indoors
- Turbulence modelling for CFD : validation, inter-comparison
- Mesh sensitivity issues for CFD

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4. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN SOURCE, RELEASE AND DISPERSION FOR LIQUID H2

EXECUTIVE SUMMARY

Modelling the release and dispersion of liquid hydrogen requires the understanding and quantification of phenomena that are different from those in the release of hydrogen in gaseous form e.g. two-phase release sources, multi-phase jets, gas behaviour at low temperatures, phase changes, pool formation and spreading, heat transfer with the surrounding environment, effect of weather conditions e.g. temperature, humidity, wind and atmospheric stability, effect of ground and roughness/obstacles configuration, and effect of turbulence and buoyancy on all the above phenomena. The quantity and the level of details of the experimental data that are available in the scientific literature are limited. The available data do not allow for the complete accurate quantification and modelling of the phenomena and for the validation of the models. Several validation analyses of CFD models in comparison with the available experimental data have been performed with different degrees of accuracy. The acceptance criteria for model performance evaluation that were developed and applied for other fields (e.g. air quality, LNG dispersion) should be revised for hydrogen because of the specific hydrogen features and behaviour. Analytical models for the whole release and dispersion process and in some cases only for specific stages of the release have been developed. Nevertheless a complete validation of those models is missing.

Liquid hydrogen is one of the possibilities that are currently under consideration for hydrogen storage and transport due to its larger density (~71 Kg/m^3 at 20 K) compared to that of compressed gaseous hydrogen (0.08 Kg/m^3 at 300 K and 101.325 kPa pressure). It was shown that when cryogenic pressure vessels for the automotive industry are filled with LH2 or CcH2 (cryo-compressed hydrogen), these vessels contain 2–3 times more fuel than conventional ambient temperature compressed H2 vessels (Aceves, et al., 2010) (Kircher, at al., 2011). For the same reason, liquid hydrogen is extensively used in rocket applications and it is considered one of the most promising solution for the future of aviation (Janic, 2010) (Frischauf, et al., 2013) (Khandelwal, et al. 2013). According to Tzimas, et al. (Tzimas, et al., 2007), between 3000 and 8000 LH2 road tankers could be required to deliver LH2 to fuelling stations in Europe by 2050. The technical and economy feasibility of a CO2 free hydrogen chain was confirmed in a recent study (Yasushi Yoshino, 2013). In that study, it is foreseen the hydrogen production and liquefaction in Australia and subsequent LH2 transport via ship (238500 tons per year) from Australia to Japan. In the ICEFUEL cable study (integrated cable energy system for fuel and power), they investigate the possibility of delivering LH2 and superconducting electric power simultaneously in the same cable to the customer (Friedrich et al., 2012). In this context in order to handle large quantities of LH2 it is crucial to develop and validate models that can help to predict the consequences of potential liquid spills. LH2 spills generate very large volume of GH2 since the LH2 density at 20 K and one atmosphere is 70.8 Kg/m^3 while the GH2 density at 300 K and one atmosphere is 0.089 Kg/m^3. Therefore 1 litre of LH2 can produce more than 850 L of gas under NTP. The hydrogen dispersion and mixing in air forms a flammable cloud that in case of ignition can generate a large overpressure or a fire, depending on the local conditions. It must be emphasized that a cloud resulting from LH2 spill will be dispersed more slowly and will remain closer to the ground for a longer time compared to a cloud from a CH2 leakage at an ambient temperature and pressure because of different buoyancy behaviours. The density of cryogenic hydrogen is much larger than the density of hydrogen at ambient temperature and pressure (ρ_{H2}= 0.08 Kg/m^3 at 300 K, ρ_{H2}= 1.3 Kg/m^3 at 21 K). The longer the flammable cloud stays close to the ground the more likely is that it will be ignited.

Other major hazards related to LH2 are the very low temperature (20.28 K) which can cause severe tissue (burns) frostbite and the enhanced embrittlement of material (Rigas and Sklavounos, 2005) but the modelling of those 2 effects will not be considered in this report.

STATE OF THE ART

According to the Pritchard and Rattigan' position paper (2010), "applications involving liquid hydrogen present additional fire and explosion hazards to those arising from use in gaseous form, which need to be fully appreciated if levels of safety comparable to those from conventional fuels such as petrol and liquefied petroleum gas are to be achieved". They also add that "the consequences of an accidental spillage or leak of liquid hydrogen are poorly understood, particularly the initial stages of pool spread and vaporisation. A better understanding of this initial phase together with more experimental data on the dispersion phase are required if reliable models for predicting the consequences are to be developed and validated." Their conclusions are consistent with the findings of another investigation where the authors identified gaps of CFD modelling of accidental hydrogen release (Baraldi, et al., 2011). In that report, it was highlighted that a limited number of experiments of LH2 spillages are available in the scientific literature (Witcofski and Chirivella, 1984), (Chirivella and Witcofski, 1986), (Schmidtchen, et al., 1994) (Dienhart 1995), (Verfondern and Dienhart, 1997, 2007) (Nakamichi, et al., 2008). Because of safety reasons, liquid helium was used as replacement for liquid hydrogen by Proust and co-workers (Proust, et al., 2007). More recent experiments of liquid hydrogen spillage were carried out at HSL/HSE (Royle and Willoughby, 2011) (Hooker, et al., 2011). Their experiments provide a further confirmation that a pool can be formed if a liquid release is made on the ground and the ground surface is sufficiently cooled. Moreover oxygen and nitrogen freeze, forming a solid deposit on the ground. Friedrich et al. (Friedrich, et al., 2012) performed experiments of release and combustion of cryogenics hydrogen jets, providing an estimate of safety distances and an extrapolation model for other jet conditions.

In general in the experiments in the literature, mainly the LH2 release and dispersion are investigated while experiments with the entire sequence of release and dispersion followed by explosions and/or fires are rare (Hooker, et al., 2005).

Several physical phenomena have to be modelled in numerical simulations in order to describe accurately the LH2 release and dispersion: two-phase release sources, multi-phase jets, gas behaviour at low temperatures, phase changes, pool formation and spreading, heat transfer with the surrounding environment, effect of weather conditions e.g. temperature, humidity, wind and atmospheric stability, effect of ground and roughness/obstacles configuration, effect of turbulence and buoyancy on all the above phenomena.

Schmidt et al. (1999) performed CFD simulations of the experiments that were carried out at BAM (Schmidtchen, et al., 1994). They assumed a pure gas release and their conclusions was that "The agreement of these results with the experiments is still not as it would be desirable. This is to a certain extent certainly due to the restrictions of the calculations to gas release, but not only." The requirement for extended and systematic experimental campaign is stated in their paper.

In Statharas, et al. (2000) the results of CFD simulations of experiments with a release rate of 0.37 kg/s are described. By including the heat transfer to the ground in the model the agreement between experiments and simulations was significantly improved and the maximum concentration was in most cases predicted within a factor 2. Several years later, Venetsanos and Bartzis (Venetsanos, et al., 2007) used the same CFD model (ADREA-HF) to investigate the effect of some parameters in reproducing the NASA experiments (Witcofski and Chirivella, 1984), (Chirivella and Witcofski, 1986) with a release rate of 9.5 kg/s. By modelling the source as a two-phase jet (compared to a pool) and including the heat transfer to the ground, the best agreement between experiments and simulations was achieved. Nevertheless some discrepancy was still observed in some measurement sensors and that was attributed to wind meandering that was not modelled in the simulations and to a low value of the heat flux from the ground. Reproducing the correct wind field and setting the correct boundary conditions in terms of temperature and humidity both of the soil and of the air is the initial challenge that is essential for the results accuracy of the simulations, even before the hydrogen release starts. Few years later Venetsanos (Baraldi et al., 2009) applied the same CFD modelling strategy to the numerical analysis of LH2 release and dispersion in a mock-up re-fuelling station, investigating the effect of wind direction and the presence of an obstacle on the flammable mass and volume. The NASA experiments (Witcofski and Chirivella, 1984), (Chirivella and Witcofski, 1986) were also used for validation of a LES method (Molkov, et al., 2005).

Another challenge in performing numerical simulations of LH2 release and dispersion is the modelling of the source term since observations indicate that the flow is already two-phase at the exit orifice (Schmidtchen, et al., 1994) (Statharas et al., 2000). In their CFD analysis of the HSL /HSE experiments (Hooker, et al., 2011) (Royle and Willoughby, 2011) (release rate =0.071 kg/s) with the FLACS code, Ichard, et al. (2012) performed a sensitivity study, increasing the gas volumetric fraction of the source term from 0.76 to 1. They achieved the best agreement between experiments and simulations with a value equal to 0.99. In a previous study with the FLACS solver by Middha and coworkers (Middha, et al., 2011), the simulated maximum concentrations were within a factor of 2 compared to the experimental data. They also investigated the effect of the atmospheric stability on the simulation results, achieving a better accuracy with the stable atmospheric class. Sklavounos and Rigas validated the CFX solver (Sklavounos and Rigas, 2005) against the NASA experiments, also producing simulation results within a factor 2 of the observed values. Recently Jaekel and colleagues (Jakel, et al., 2012) used the ANSYS-CFX v.13 to perform a validation study against the HSE/HSL experiments (Hooker, et al., 2011). Also in their investigation they carried out a sensitivity study on the percentage of liquid and gas hydrogen at the source term considering a fraction of liquid hydrogen of 100%, 75%, 50% and 25% of the release mass flow. They achieved the best agreement with the experiments in term of pool distribution with 75% and 50%. Nevertheless the authors stated that the temperature distribution at the wall and the pool front velocity were not in the range or close by the experimental data and that they need further investigation.

Chitose, et al. developed in the 90s the multi-phase hydrodynamics analysis code to investigate a large scale LH2 dispersion. Ishimoto et al. (2008) uses CFD to estimate the thermodynamic effect on the LH2 jet atomization process of a LH2 jet such as liquid column interfacial instability, break-up of the jet column, formation of liquid film and generation of droplets. This work has not yet been validated against experiments.

Beside CFD studies, analytical mathematical models were also developed to describe specific stages of the liquid hydrogen release. Kim and co-workers (Kim, et al., 2011)(Kim, et al., 2012) applied perturbation techniques to solve a simple physical model that describe the LH2 pool spreading. They found that the perturbation method yields nearly identical results to the numerical solution when third order perturbation solutions are considered for the pool volume. The dimensionless governing parameter is the evaporation rate. Epstein and Fauske developed a top-hat jet/plume model to obtain simple closed-form expressions for the total mass and volume of the flammable cloud for a gas or volatile liquid release (Epstein and Fauske, 2007).

Harstadt and Bellen (2006) investigated the vaporization of a LH2 pool and developed some analytical expression for the minimum pool evaporation time for the H2 film-boiling rates. Verfondern and Dienhart (2007) developed a computer model LAUV to simulate the spreading and vaporization of a cryogenic liquid under various conditions e.g. different grounds (solid or water) showing a satisfactory agreement between the model results and the experimental data.

A homogeneous non-equilibrium, two-phase, critical flow model, the homogeneous direct evaluation model (HDE), was developed from first principal thermodynamics and equation-of-state formulations by Travis et al. (2012). The model was validated with NASA cryogenic data for liquid and supercritical hydrogen, methane, nitrogen, and oxygen in terms of critical mass fluxes for a range of stagnation conditions.

Houf and Winters developed a series of models to describe the whole release process of a small and slow leak (at very low Mach number) from a LH2 storage system (Houf and Winters, 2011). They divided the release process in 4 zones: a leak model followed by 3 turbulent entrainment models. Equilibrium thermodynamic models based on the NIST REFPROP subroutines (Lemmon, et al., 2007) are used to predict the state of leaking hydrogen and the state of hydrogen-air mixture. In a more recent paper, the two authors (Winters and Houf, 2013) developed a similar multi-zones model for high-pressure liquid release, adding a model for the zone of under-expanded flow (Mach number >1). The only validation that is shown in the papers is for the model for gaseous hydrogen leaks, demonstrating a favourable agreement between the model results and the experimental data for hydrogen concentration along the centreline.

Li and colleagues used the PHAST software to calculate the harm-effect distances of LH2 releases (Li, et al., 2012) and of cryo-compressed hydrogen releases (Li, et al., 2013). Their analysis and results have a high level of uncertainties because PHAST is based on simplified models and correlations that do not take into account all the relevant parameters, and are not valid for all range of possible conditions and hazardous materials. The authors themselves state "The code package PHAST applied is principally developed for releases of natural gas. Whether the code can be applied for hydrogen releases need further investigation" (Li, et al., 2013). Although the authors show some validation for hydrogen gas release, the release is only one of the many phenomena that are considered in their investigation (cold clouds, jet fires, flash fires, explosions) without showing any validation.

The CFD capabilities of predicting hydrogen concentrations seem to be accurate within a factor 2 in some analyses (Statharas et al., 2000) (Sklavounos and Rigas, 2005) (Middha et al., 2011). Although a factor 2 is considered as an acceptable criteria for model performance evaluation in other fields e.g. air quality (Chang and Hanna, 2004), and LNG dispersion (Ivings et al., 2013) for the specific applications of hydrogen release a factor 2 could not be acceptable. Overestimating or underestimating hydrogen concentrations by a factor 2 can cause a much larger discrepancy in the calculations of the overpressures that are generated by the combustion. If one compares the state of the art for LNG and LH2 releases, it seems that the LNG research reached a more advanced state from the point of a model evaluation procedure, including the definition for acceptance criteria a validation matrix for model performance evaluation. For LNG it exists already a Model Evaluation Protocol for assessment of models for dispersion: "the protocol comprises scientific evaluation of the numerical and physical basis of models for the dispersion of LNG vapour, model verification, and validation; resulting in a comprehensive model evaluation report which includes qualitative and quantitative criteria for model acceptance. A supporting suite of validation data, and guidance on the use of this data, has also been produced" (Ivings, et al., 2013). The FCH JU funded SUSANA project is starting in 2013 with the target of developing a Model Evaluation Protocol for hydrogen, including a validation matrix for CFD simulations.

IDENTIFICATION OF KNOWLEDGE GAPS

Several open issues still exist in modelling liquid hydrogen releases for safety analysis:

- Two-phase release
- Multi-phase jets.
- Dispersion of cryogenic and LH2 in enclosures with passive and forced ventilation

- The physical properties of liquid hydrogen and gaseous hydrogen at very low temperature (but also of O2 N2, H2O – close to saturation) including differences with the ideal gas law.
- Phase change issues such as the hydrogen evaporation and the condensation and solidification of nitrogen, oxygen, and water in the air.
- Effect of weather conditions on the release e.g. humidity, temperature, wind speed and direction, atmospheric stability class.
- Conductive, convective and radiative heat transfer between the cold hydrogen and the surrounding environment including air and the ground.
- Effect of buoyancy and turbulence on the above phenomena.
- The lack of experiments that can close the above open issues is a major obstacle to the development, validation, and application of numerical tools.

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5. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN ACCIDENTAL IGNITION

EXECUTIVE SUMMARY

It has been demonstrated experimentally and numerically that accidental releases of pressurised hydrogen are prone to spontaneous ignition. The actual causes of ignition could include (1) electrostatic and corona discharge; (2) mechanically generated sources; (3) diffusion ignition due to shock heating and (4) catalytic ignition. It is also recognised that two or more of these mechanisms could be present together. Key advances on these topics can be summarised as follows:

Electrostatic and corona discharge: Experimental investigations have confirmed the possibility of hydrogen-air mixtures being ignited by corona discharges in certain situations while the corona discharges which would ignite the released hydrogen were thought to be unlikely in horizontal releases of hydrogen close to ground level. A typical hydrogen application will unlikely have the quantity of particulate present internally to generate corona discharges of sufficient energy to cause ignition. The ignition possibility by electrostatic discharge may be reduced by using a tapered porous outlet.

Mechanically generated sources: The limiting power densities for friction processes using mild and stainless steels have been established for only 10% and 30% hydrogen in air mixtures. The limiting values in 10 % hydrogen/air mixtures were found to be lower than those in 30 % hydrogen; and the limiting power densities for stainless steel are lower than those for mild steel.

Diffusion ignition: Numerical simulations have demonstrated that direct releases of pressurised hydrogen into the air could result in spontaneous ignition if the rupture rate is assumed to be infinitely fast. But there have been no experimental observations or further numerical studies to demonstrate that such ignition could sustain a jet flame.

Both experimental and numerical results suggested that the propensity to spontaneous ignition increases with the increase in reservoir pressure, tube diameter and length. As the tube length increases, the minimum release pressure required to trigger a spontaneous ignition was found to decrease that indicates appearance of ignition at some distance from the membrane. The rupturing rate of the bursting disks or the pressure boundary in the numerical simulations was also found to be of influence.

Ignition of hydrocarbon-hydrogen-air mixtures: Experimental investigations have identified that at temperatures less than 1050 K, the addition of hydrogen to hydrocarbon-air mixtures could increase the spontaneous ignition delay and vice versa for temperatures above 1050 K.

Catalytic ignition: Experimental investigations have demonstrated that catalytic ignition of leaked hydrogen gas within an enclosure can be initiated with or without surface heating.

STATE OF THE ART

The JRC 2011 Reference Report on "Prioritisation of Research and Development for modelling the safe production, storage, delivery and use of hydrogen" already contains description of the research carried out up to that review point. For completeness, some of the earlier work already included there will still be briefly mentioned in the present review while more detailed discussion will be given to relevant research published after the report.

It is now widely accepted that accidental releases of pressurised hydrogen are prone to spontaneous ignition. Astbury and Hawksworth (2007) postulated four potential ignition mechanisms: the reverse Joule–Thomson effect, the electrostatic ignition, diffusion ignition

(ignition behind a shock wave) and hot surface ignition of generated by mechanical sources. They also recognised that two or more of these mechanisms could be present together. Subsequent research has ruled out the reverse Joule–Thomson effect as a potential trigger for spontaneous ignition but found evidence of all the others. The majority of the published body of research has focused on diffusion ignition while there are few papers which addressed ignition by the electrostatic ignition or hot surfaces.

Ignition by electrostatic discharge

Hooker, et al. (2011) experimentally investigated electrostatic ignition by corona discharge and found that hydrogen-air mixtures can be ignited by corona discharges of the type that might be produced where fine particles are a potential of several tens of kilovolts above the surrounding atmosphere. Such situations could be expected at the top of tall vent stacks, tens of metres above ground, in the presence of large atmospheric electric fields (e.g. during snow fall). Corona discharges which could ignite the released hydrogen were thought to be unlikely in horizontal releases of hydrogen close to ground level. They also found that dispersion of dusts up to 160 g with hydrogen released from 20 MPa did not appear to generate hazardous electric fields in terms of corona discharges. Merilo, et al. (2012) conducted a series of tests with an isolated plate in close proximity to a grounded probe and found that even a small quantity of entrained particulates could be a source of spontaneous ignition by electrostatic discharge. They believed that both electrostatic discharge and corona discharge could be responsible for some of the ignition that occurred in their tests. In some of their tests, it was found that even with large quantities of iron oxide particles entrained in the hydrogen jet and while a sharp-pointed ungrounded conductor was charged to a high potential no ignition occurred. They made the observation that brush discharge sufficient to cause ignition might be unlikely due to the quantity of particulates required to generate the high electrostatic potential.. Hence, it is unlikely that entrained particles would be the source of ignition in common applications. This is consistent with the findings of Hooker, et al. (2001).

Imamura, et al. (2009) investigated the ignition possibility of hydrogen by electrostatic discharge at a ventilation duct outlet. They investigated the effect of the outlet shape using four types of outlets including 6.35, 12.7 and 25.4 mm diameter pipes and a tapered porous outlet which was referred to as TP outlet. Iron (III) oxide particles were used as the model dust. It was clarified that if the ventilation duct outlet is grounded, few electrostatic charges were generated on the ventilation duct outlet. But it was also found that not all generation of electrostatic charges from the mixture of hydrogen and iron oxide can be removed by grounding only. Even so, the voltage and energy of the mixture at a certain downstream position were found to be reduced by using the TP outlet. Their results imply that the ignition possibility by electrostatic discharge may be reduced by using the TP outlet.

Ignition by mechanically generated sources

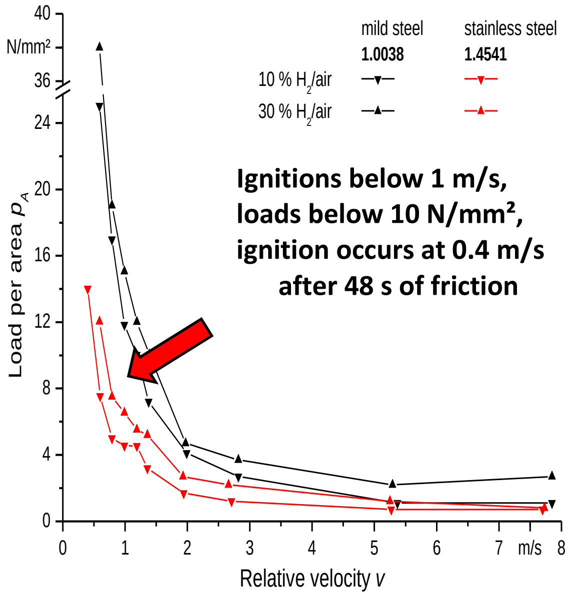
Welzel, et al. (2011) investigated ignition by mechanically generated sources for two different hydrogen/air mixtures. For friction processes, two ignition sources can be generated simultaneously, i.e. hot surfaces and mechanically generated sparks. It was found that ignition is possible even below a velocity of 1 m/s. They identified limiting power densities for the ignition of 10% and 30% hydrogen/air mixtures (Figure 5.1), for friction processes involving mild and stainless steels. Limiting values for ignition in 10 % hydrogen/air mixtures are lower than those in 30 % hydrogen; and the limiting power densities for stainless steel are lower than those for mild steel.

Diffusion ignition – experimental investigations

Since Wolanski and Wojciki's (1972) pioneering experiments of diffusion ignition nearly 40 years ago, little work was done until recent. More recent experimental studies have been conducted to demonstrate diffusion ignition of pressurized hydrogen release through a length of tube almost simultaneously by Dryer, et al. (2007), Golub, et al. (2007, 2008, 2009a, 2009b), Mogi, et al. (2008, 2009), Desilet, et al. (2009), Grune, et al. (2011), Kitabayashi, et al. (2012) and Lee, et al. (2011). While there were variations in the experimental set up, the releases all passed through a tube and burst disk that initially separated the pressurized hydrogen and air at atmospheric pressure. Both Golub, et al. (2008) and Mogi, et al. (2008) found that the minimum release pressure required for spontaneous ignition to occur depends on the tube length and diameter. The type of the bursting disks was also found to be of influence. In general, the experimental results suggested that the propensity for spontaneous ignition increases with the increase in reservoir pressure, tube diameter and length. As the tube length increases, the minimum release pressure required to trigger a spontaneous ignition decreased. Most of the investigators used circular tubes while Golub, et al. (2008, 2009a) used both circular and rectangular tubes.

Their results suggested that the cross section shape of the tube is of importance. They showed experimentally that at the same cross section area the spontaneous ignition in narrow rectangular tube occurred at lower reservoir pressure than in round tubes. At an initial reservoir pressure of 1.5–2 MPa, spontaneous ignition was found to occur with the rectangular tube. Using photodiode signals and flame images, Lee, et al. (2011) observed the propagation of a flame inside the tube. They detected flame near the rupture disk as the bursting pressure increases. However, when the tube length was not sufficiently long, a flame was observed only in the boundary layer at the end of tube and it quenched after exiting the tube. It was hence postulated that the formation of a complete flame across the tube is important to initiate an ignition which can sustain a diffusion flame after jetting out of the tube into the air.

Recent tests of Kitabayashi, et al. (2012) used various lengths of tubes up to 4.2 m filled with air at ambient pressure. The storage pressure sufficient for spontaneous ignition was found to be a function of the tube length with characteristic minimum at about 3.8 MPa for tubes with 10 mm internal diameter. Below this critical diaphragm bursting pressure and with longer or shorter tubes than the length of about 1100 mm, no ignition was observed.



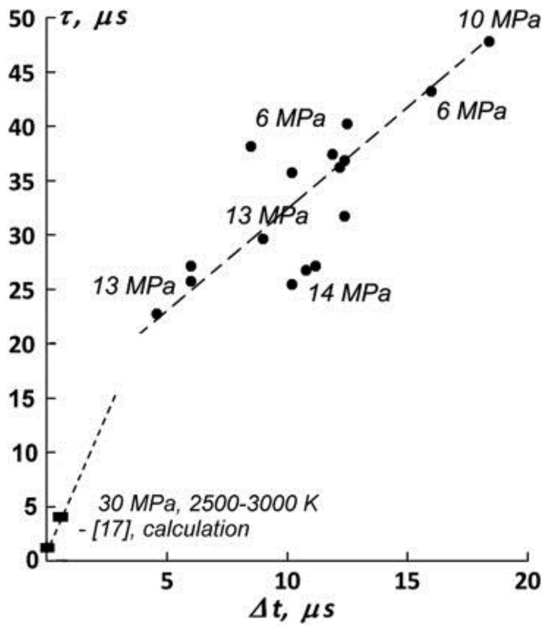


Figure 5.1. Left: Ignition of hydrogen/air mixtures by mechanically generated ignition sources (reproduced from Welzel, et al., 2001)). Right: Dependence of self-ignition delays of hydrogen τ on the rupture rate of the diaphragm Δt *(reproduced from* Golovastov and Bocharnikov, 2012).

Golovastov and Bocharnikov (2012) experimentally studied the influence of the rupturing process on spontaneous ignition resulting from a pulse discharge into an air filled open channel. The diffusion spontaneous ignition of hydrogen is defined both by initial pressure of hydrogen and by rupture rate of the diaphragm. The faster a shock wave is formed the faster ignition is started. In the range of initial pressures 5.0–14.0 MPa the rupture rate of the diaphragm was varied from 5 to 20 μs. Figure 5.1 (right) shows the measured delay of ignition of hydrogen τ discharged into the channel at different durations of the opening Δt. More rapid opening of the diaphragm accelerated the formation of a shock wave and led to rapid heating of the air behind the shock wave front. The given dependence was found to have monotonic nature and practically did not depend on initial pressure in the range indicated. Ignition delay can be decreased to 23 μs behind the shock wave for the shortest opening duration experimentally studied here. These findings are in line with the numerical predictions of Xu, et al. (2009b) for release into air without channel.

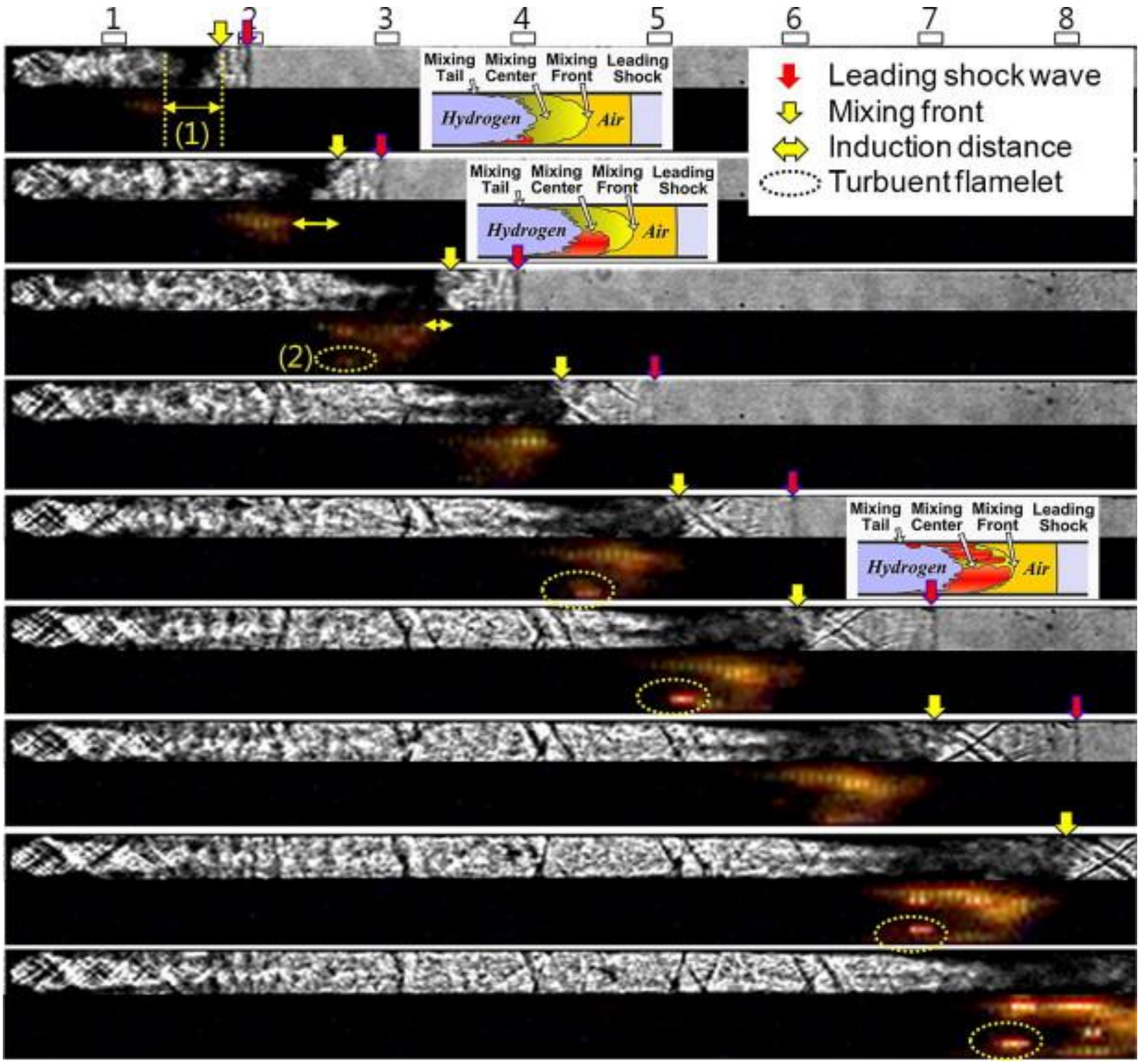


Figure 5.2. Spontaneous ignition and the flame propagation at the burst pressure of 9.0 MPa, measured shock wave speed is 1400–1500 (average 1460) m/s, theoretical shock wave speed is

1483 m/s, (1) induction distance between the mixing front and flame front; (2) turbulent flamelets occasionally shown at the boundary layer (reproduced from Kim, et al., 2012)

In the recent flow visualization study of Kim, et al. (2012) shown in Figure 5.2, the initial ignitions were observed at the mixing spot in the boundary layer of the mixing zone. The flame ignited at the boundary layer follows up the mixing front and spreads to the mixing tail of the mixing zone as the shock wave moves downstream. The glinting of the flame along the boundary layer led them to assume that it was turbulent.

Dryer, et al. (2007) provided further insight revealing that the internal geometry downstream of the bursting disk greatly affected the likelihood of spontaneous ignition, especially for relatively low release pressures. This led to the postulate that the bursting disk rupture process has an important influence on mixing and ignition through multi-dimensional shock formation, reflection and interactions. However none of the experimental groups investigated in detail the influence of different internal geometries while this aspect has been the subject of several numerical simulations.

Diffusion ignition – numerical studies

Numerical investigations were performed by Brady and Sung (2010), Bragin and Molkov (2009a, 2009b, 2011), Golub, et al. (2007, 2008, 2009a, 2009b), Lee and Jeung (2009) (2009), Radulescu, et al. (2007), Shen and Sun (2012), Wen, et al. (2009), Xu, et al. (2008, 2009a, 2009b, 2011, 2012) and Yamada, et al. (2009a, 2009b, 2011). The earlier numerical simulations of Liu, et al. (2006) and Xu, et al. (2008) revealed the possibility of spontaneous ignition even when hydrogen is directly released into air. However, their results need to be interpreted in the context that the release was assumed to be infinitely fast. Xu, et al. (2010) also investigated the effect of a thin flat obstacle on the spontaneous ignition of a direct pressurized hydrogen release. For the conditions studied where the obstacle considered was a thin round disk having a diameter that is twice of the leak opening diameter "D" and placed at distance of 1D, 2D and 3D above the leak point, they found that the presence of the obstacle plays an important role in quenching the flame following spontaneous ignition. In reality, any controlled release or release caused by equipment failure occurs at a finite rate. As revealed in the subsequent numerical and experimental studies, the rupture rate has important influence on the propensity to spontaneous ignite.

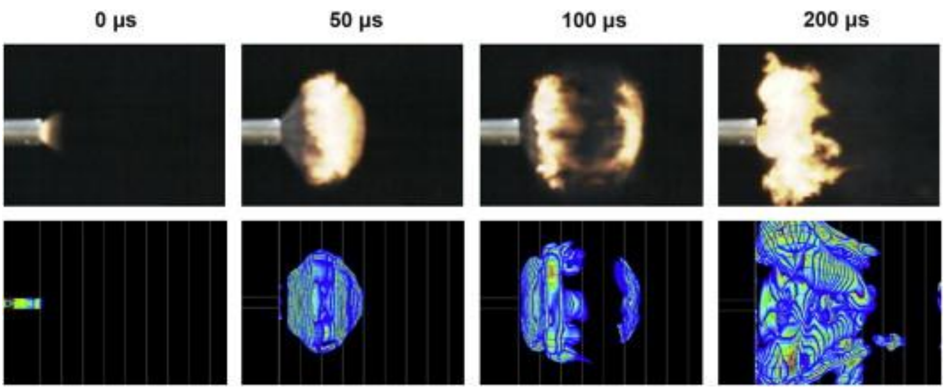


Figure 5.3. Comparison of high-speed video camera experimental photographs obtained by Mogi, et al. (2008) with numerical LES snapshots (reproduced from Bragin and Molkov, 2009b).

Any accidental releases, in practice, would often involve releases through a section of a tube. These were also the configurations used in almost all the aforementioned experimental studies. Largely due to this reason, most subsequent numerical studies have focused on this type of release scenarios. The independent studies of Bragin and Molkov (2009a, 2009b, 2011), Golub, et al. (2007, 2008, 2009a, 2009b), Koichi and co-workers (Yamada, et al. 2009a, 2009b, 2011), Wen, et al. (2009) and Xu, et al. (2008, 2009a, 2009b, 2011, 2012) have all identified that the air behind the leading shock is shock-heated and mixes with the released hydrogen in the contact region.

Ignition is firstly initiated inside the tube and then a partially premixed flame is developed. It was thought that shock-heated air and the partially premixed flame are two major factors providing the potential energy to overcome the under-expansion and flow divergence following spouting from the tube. Yamada, et al. (2011) also identified a shock in the tube under certain conditions as well as the generation of vortices behind the shock wave in a long tube. From the latter they postulated the possibility of spontaneous ignition induced by vortices. Parametric studies conducted by Wen, et al. (2009) revealed that the rupture process induces significant turbulent mixing at the contact region via shock reflections and interactions. Further work (Xu, et al. 2009b) showed that slower rupture times and lower release pressures led to increases in ignition delay time and hence, reduces the likelihood of spontaneous ignition. It was found that if the tube length is smaller than a certain value, even though ignition could take place inside the tube, the flame is unlikely to be sufficiently strong to overcome under-expansion and flow divergence after spouting from the tube and hence is likely to be quenched. These results were later confirmed by the experimental work of Golovastov and Bocharnikov (2012).

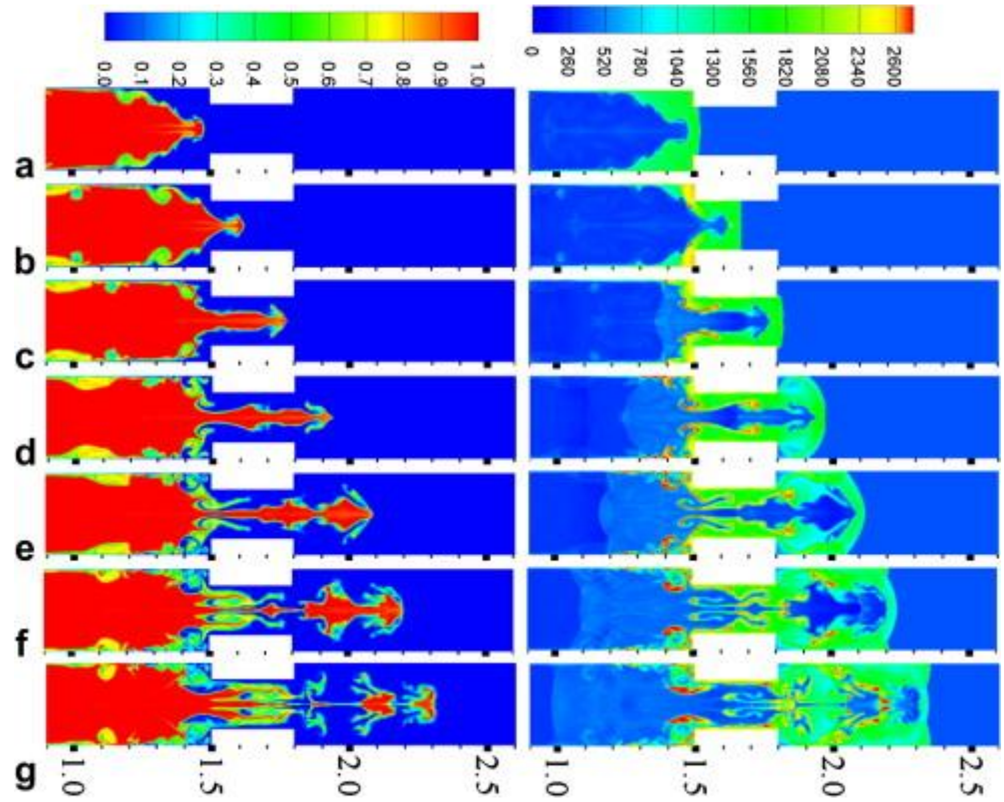


Figure 5.4. Calculated contours of Logarithm of hydrogen mass fraction in the left column and temperature (K) in the right column at a time interval of 1 μs starting from 13 μs for the case of 50 bar (length unit in cm) (reproduced from Xu, et al. 2012).

Bragin and Molkov (2009a, 2009b) numerical simulation showed the transition Bragin and Molkov (2009a, 2009b) numerical simulation showed the transition from spontaneous ignition inside of the tube to a sustained jet flame. As shown in Figure 5.3, they reproduced the experimentally observed phenomenon of flame separation. They suggested the transition to a sustained jet flame is dependent on the initial jet formation stage, where the developing annular vortex entrains the combusting mixture into the recirculation zone. Once the flame is stabilized near the tube exit, it acts as a pilot flame and ignites the jet flame.

Inspired by the comment of Dryer, et al. (2007) about the effect of internal geometry, Xu, et al. (2012) investigated the effect of local contraction within the tube. As shown in Figure 5.4, they found that a local contraction can increase the propensity for spontaneous ignition and enhancing turbulent mixing from shock formation, reflection and interaction.

Diffusion ignition – Theoretical studies

Maxwell, et al. (2013) conducted a series of experiments designed to examine the role of turbulent instabilities on the ignition process of pressurized hydrogen jets which are released into oxidizing environments. Despite the presence of confinement in the experiments, the ignition limits determined experimentally were found to be in general agreement with the trends of previous work by Maxwell and Radulescu (2011). This previous work was a 1-D numerical model of a release into an unconfined environment. The role of confinement in the experiments was found to influence ignition at lower limits compared to the 1-D ignition model, and also promote turbulent mixing through shock reflections and flow instabilities. They concluded that turbulent mixing influences how the ignition spots interact to ignite the entire jet.

Ignition of hydrocarbon-hydrogen-air mixtures

Frolov, et al. (2013) conducted numerical simulations using detailed chemistry on the effect of hydrogen addition on the propensity for spontaneous ignition of homogeneous and hybrid mixtures of heavy hydrocarbons in air. Reactivity of hydrogen-containing mixtures is not always higher than that of pure hydrocarbon air mixtures. At temperatures less than 1050 K, the addition of hydrogen to such mixtures was found to increase the spontaneous ignition delay. At temperatures exceeding 1050 K, hydrogen addition was found to decrease the overall spontaneous ignition delay thus indicating that hydrogen acts as a promoter.

Catalytic ignition

In order to determine potential fire safety hazards associated with hydrogen release in the presence of a catalyst, Brady, et al. (2010) experimentally investigated the ignition characteristics of lean pre-mixed hydrogen/air mixtures using a stagnation-point flow configuration against a platinum surface. They observed two distinct regimes - catalytic surface reactions and gas-phase ignition. They demonstrated that depending on mixture equivalence ratio (a measure of mixture fraction), catalytic surface reactions can be initiated with or without surface heating. When sufficient surface heat is released via exothermic catalytic reactions, gas-phase ignition can occur, increasing the apparent danger of hydrogen leaks in the presence of a catalytic surface. Their findings indicate that ultra-lean hydrogen/air mixtures can be catalytically ignited even in the absence of external heat addition. This suggests that a hydrogen leak in the presence of a catalytic surface may pose a fire safety risk even at room temperature. Further experimental investigations by Brady, et al. (2012) indicated that for all conditions studied, catalytic ignition was observed when the hydrogen comes in contact with the catalytic surface, which was initially at or near room temperature. After ignition, these surface reactions led to steady state surface temperatures in the range of 600 to 800 K.

IDENTIFICATION OF KNOWLEDGE GAPS

Past research on accidental ignition of hydrogen releases have been carried out by fragmented research groups in the United Kingdom, United States, Germany, Japan, Korean, Russia and China. Despite the progress made, the lack of coordination has resulted in knowledge gaps which need to be filled through a systematic approach involving carefully designed experiments to validate predictive tools which can then be used to conduct numerical calculations with the view to establish ignition potential for a range of release scenarios that are of significance to the introduction of hydrogen as an energy carrier into the economy. Furthermore, the following conditions have been largely overlooked and their propensity to spontaneous ignition needs to be given high priority:

- The release through non-circular openings (smooth and with sharp edges), either direct into the air or through a section of tubes;

- Spontaneous ignition in complex geometries, e.g. after pipe bends, etc.
- Simulation of real opening of a rupture disk with moving mesh;
- Parameters of valve opening that eliminates ignition;
- The release of hydrogen blended with hydrocarbon fuels;
- Thorough validation of numerical predictions with flow visualization data;
- Numerical calculations with validated predictive tools for a range of systematically defined release scenarios including variations in reservoir pressure, exit shape and dimension, tube length, internal geometry with the tube, etc. to establish an ignition probability database for use by industry;
- The ignition propensity of hydrogen-air mixtures by mechanically generated sources at different concentrations;
- The ignition propensity of hydrogen blended hydrocarbon fuel-air mixtures by mechanically generated sources at different concentrations; and
- The ignition propensity of hydrogen blended hydrocarbon mixtures by electrostatic and corona discharge at different concentrations.

It is believed necessary to involve stakeholders closely to initiate a co-ordinated research programme to address the above issues though collective funding from the European Commission, the US Department of Energy and other national funding bodies in countries where capabilities have been established as demonstrated in the review above.

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6. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN COMBUSTION

EXECUTIVE SUMMARY

Depending on the hydrogen-air mixture characteristics, such as concentrations, temperature, pressure, etc., and flow geometry, combustion process can undergo strong flame acceleration and/or even deflagration-to-detonation transition (DDT). These regimes are usually characterized by high burning rates and consequently by high pressure loads, which can be potentially dangerous for life and property.

Despite many years substantial achievements in the area of the flame acceleration and DDT, still many specific aspects of the problem remain unclear. Dependence of the potential danger of the combustion process appeared to be very sensitive to the geometrical conditions of the processes, mostly to the confinement and to the congestion of the volume. Currently a unified physical model and corresponding numerical instrument which can be used over the entire range of phenomena is not available. Numerous combustion models are usually addressing only specific regime or phenomenon and are applicable only in their domain of validity. Detailed clarification of the combustion physical nature and creation of the simplified engineering models for the separate phenomena as well as comprehensive numerical models, allowing predictively simulate the whole sequence of events during possible accident is a continuing challenge for the researchers.

This chapter summarizes briefly some of the activities in the key directions which have been made in the recent period. In the report (Baraldi, et al., 2011) of the previous workshop organized by JRC IET in October 2009, the knowledge gaps in CFD modelling were addressed, and many of them still remain actual (see e.g., (Jordan 2009; Kotchourko 2009; Molkov 2009), therefore only new issues were included into state-of-the-art description, however the remaining knowledge gaps are listed in the concluding section.

STATE OF THE ART

Confinement

As it was found already in the early studies (e.g., Chan, et al., 1983; Kumar, et al., 1989; Pfortner, et al., 1983), the possibility of premixed flame to accelerate and therefore finally be dangerous, is very sensitive to the confinement of the volume. The combustion of the fully confined volumes is relatively good understood and its effects can be reasonably predicted by modern combustion models (Baraldi, et al., 2011).

The necessity to take into account more practical configurations initiated consideration of the combustion in the volumes with one or more vent areas of the varying shapes. Starting with the channel-like experiments (Sherman, et al., 1989) it was shown that transverse venting can substantially reduce flame speed and in case of detonation even cause its failure. Further results of the influence of the transverse and longitudinal venting were obtained by several research groups (Ciccarelli, et al., 1998; Alekseev, et al., 2001; Alexiou, et al., 1997) and the criteria for the evaluation of the flame acceleration potential were proposed (Dorofeev, et al., 2001). These criteria have significant practical importance as it can be directly used for the risk evaluation for concrete configurations such as tunnels, which were experimentally and numerically (e.g., Baraldi, et al., 2009) studied. Further extension of the vent influence studies involved investigation of the semi-confined volume, such as horizontal flat layer of the H_2 distribution limited from top (Friedrich, et al., 2007; Kuznetsov, et al., 2010; Kuznetsov, et al., 2011; Grune, et al., 2013). Their efforts introduced new engineering correlations which allow to evaluate hazards of the flame acceleration and detonation propagation in the flat layers of hydrogen-air mixtures.

Further deepening of the knowledge of the role of overall confinement is highly demanded due to the raised likelihood to meet such conditions in the accidental conditions. Alternative practically important configuration, which was not studied, is a one-side bounded semi-confined vertical flat layer. Such configuration can be easily realized when, for example, a jet impinges vertical wall and flows along the wall. Clarification of the possibility of the strong flame acceleration and DDT in the fully unconfined space as a limiting case (recent example (Mogi, et al., 2011) still waits for the augmented attention.

Another practically important phenomenon is vented deflagration where a number of different factors (e.g. enclosure size and geometry, vent size and inertia, relative ignition location, etc) can affect the resulting pressure loads. Experimental data of different scales and boundary conditions (e.g., Pasman, et al., 1974; Kumar, et al., 1989; Carcassi, et al., 1994; Lowesmith, et al., 2011; Kumar, et al., 2006; Daubeck, et al., 2011) and theoretical models are available in the literature. Proposed by NFPA standard (NFPA 68, 2007) on vent sizing is basically focused on the natural gas and in (Daubeck, et al., 2011; NFPA 68, 2007; Molkov, 2008) it was found that the model is over-conservative and for the stoichiometric hydrogen mixtures is not directly applicable. In (Molkov, et al., 1999) an alternative correlation for evaluation of the vent size for the enclosures without obstacles based on turbulence generated during venting was proposed. Later Jallais (2011) has shown that the recommendations from (Molkov, et al., 2008) have limited validity, while model of (Molkov, et al., 1999) globally provides good accuracy with slight overestimation. Most of the existing models are targeted to estimate only pressure peak disregarding other parameters, such as ignition location, obstacles, etc. The analytical expression presented in (Bauwens, et al., 2011) allows calculation of the both pressure peaks and takes into account most of above mentioned factors. In (Jallais, 2011) it is reported that the correlation is adequate for the hydrogen vented explosion volumes from 1 m^3 to 120 m^3 and hydrogen concentrations from 10% to 30% vol. In the currently ongoing EC project HyIndoor (Bauwens, et al., 2011) a systematic study of the venting methodology is undertaken and a formulation of the improved correlations and CFD numerical tools are expected to be proposed.

Accounting of the other confining factors, which can affect the resulting pressure loads, such as covering vent grid, relative localization of the vent, and particularly important vent cover inertia are additional challenges for the researches. Comprehensive overview of the state-of-the-art on explosions with inertial vent covers is available in (Molkov, et al., 2004). In accordance with it, the following knowledge gaps can be pointed out as the most significant: there are little experimental and analytical data available on the vent inertia effect; utilization of the recommendations developed for open and non-inertial vents require specific validation; there is no quantitative information on the turbulence generation by vent outflow; and; in general; the inertia may have a considerable impact on vent efficiency and should always be considered as a part of the venting system design (Cooper, 1998).

Thus for now, despite the existing models generally exhibit rather good agreement in comparison with the experimental data, the development of the complete models accounting for the whole set of the affecting factors (as, for example, mutual localization of the vent and ignition location) is still anticipated.

Congestion

Starting from the pioneering works of the 50's (e.g., Shchelkin, 1940), in many topical studies (e.g., Lee, et al., 1985) it was found that, obstructions on the path of the propagating flame can result in strong flame acceleration and DDT. Already in (Lee, et al., 1985; Shepherd, et al., 1991) it was pointed out that such phenomena (FA and DDT) are of primary importance for the practical applications, as e.g., for industry relevant appliance. In general, qualitatively, the sequence of events leading to FA is well known: hot combustion products push the gas before flame; this moving flow generates growing turbulence, as it flows over and around the obstacles; and the turbulence accelerates combustion process, thus providing positive feedback mechanism.

In numerous works it was shown that the details of the obstacle configuration can decisively influence on the regime of the combustion. One of the main parameter which is commonly used for the obstruction characterization is blockage ratio. However other geometrical characteristics can and actually affect the combustion process as well. In (Ardey, et al., 1996; Durst, et al., 1997) the different geometrical forms were studied: it was shown that turbulent hydrogen-air flames can be strongly accelerated if in a combustion chamber the obstacles both with low blockage ratio (BR << 50%, tube bundles, gridiron) and with high blockage ratio (BR > 50%, plate with rectangular opening) are used. Influence of the different obstacles configurations (including variation of blockage ratio, distance between obstacles, imitation of rough walls, etc) were studied in the works of Teodorczyk (Teodorczyk, et al., 1988; Teodorczyk, 1995). Interesting tests were performed in the vertical facility with partially obstructed channel (Cheikhravat, et al., 2007). Parametric study on the evaluation of limits for effective flame acceleration in obstructed closed geometries was carried out in (Dorofeev, et al., 2001; Dorofeev, et al., 2000).

Numerical simulation can provide additional insight into process of the flame acceleration and DDT. Deeper understanding was obtained after remarkably detailed CFD simulation presented in (Gamezo, et al., 2007); however further efforts are continuously undertaken to improve the knowledge and understanding of the role of obstacles in the combustion process advance both in the experiments and in numerical simulations. Among recent studies, for example, in (Gaathaug, et al., 2011) an onset of detonation behind a single obstacle was studied; and in (Heidari, et al., 2011) a possibility to simulate an onset of detonation using different techniques was considered. In the frames of the EC project HyPer (Brennan, et al., 2011) a study of small foreseeable releases and a possibly catastrophic hydrogen leakage followed by combustion of the resulting mixtures inside a fuel cell cabinet for a range of leak rates, blockage ratios and vents were investigated.

On the basis of the experimental work of (Friedrich, et al., 2007; Kuznetsov, et al., 2010; Kuznetsov, et al., 2011) on the flame acceleration in flat layer, an attempt to generalize utilization of the congestion characteristics using numerical simulations was made in (Yanez, et al., 2011). The correlations proposed in (Kuznetsov, et al., 2011) considers dependence on blockage ratio, distance between obstacles and layer thickness, while in the numerical experiments of (Yanez, et al., 2011) most of possibly significant geometrical parameters of the layout were taken into account: additionally to above mentioned also the vertical interval between obstacles, the height of the obstacles, and, as an auxiliary parameter, the distance from the first obstacle to the top. The obtained correlation introduces a new set of dimensionless parameters and provides noticeably higher level of the generality due to additional accounting of detailed characterization of the obstruction, though should not be used in practical applications without solid experimental validation.

Note, that the most of the studies are made for artificially created obstacle sets, such as repetitive periodic grids, circular orifices in the tubes at the constant mutual distance, etc., while the real industrial configurations will definitely include the obstacles irregularly placed in the volume with the very different characteristic sizes. It is well known that rough tubes without material obstacles inside them and even smooth tubes are able to promote FA and DDT (Urtiew, et al., 1966). It was found that consideration of the boundary layer can give practical results for unobstructed tubes (Kuznetsov, et al., 2005). Further analyses in this direction would have considerable practical outcome.

Thus, the current status is that despite broad scientific discussion and relatively wide experimental data base, it is still a challenge to make predictive forecasts of the realization of the definitive combustion regimes in the conditions close to the real industrial environments.

Mixture properties

Non-uniformities of the gas distribution can considerably affect regime of combustion in some cases leading to the strong flame acceleration with the possible DDT or to the reduction of the burning rate and finally even to the complete terminating of the process. However, only limited amount of the experimental data are available on the behaviour of the H_2 in the presence of the concentration gradients (e.g., (Whitehouse, et al., 1996; Sochet, et al., 1997). In the recent studies (Bentaib, et al., 2005) the data on the flame acceleration of lean H_2-air mixtures with vertical concentration variation and comparison of the obtained flame speeds with those in uniform mixtures were provided. Evaluation of the combustion regimes in the stratified horizontal layer of the hydrogen-air mixtures were performed in (Kuznetsov, et al., 2011; Grune, et al., 2012) and the numerical study for the corresponding regimes is presented in (Kudriakov, et al., 2013). Large scale vertically stratified mixtures were experimentally studied in (Bengaouer, et al., 2011). In (Kotchourko, et al., 2011) the results of the benchmarking of the different CFD codes on the basis of the data from (Bentaib, et al., 2005) are presented, the obtained results demonstrated that most of the available codes still exhibit the lack of the predictive capabilities in case of the complicated initial conditions which includes mixture composition non-uniformity.

Propagating of the flame can occur in laminar regime only for the short initial periods since the intrinsic nature of the flames causes their distortion and rapid development of the flame folding with considerable increase of the flame surface resulting in the enhanced burning rate. Supplementary events can promote further increase of the burning rates: when the flame is hit by a shock a Richtmyer-Meshkov instability can develop; if the flame propagates in the area with strong velocity shear Kelvin-Helmholtz instability can occur; reflections of the acoustic waves from the confinement leads to the acoustic-parametric instabilities; gravitation or sudden acceleration on the interface between fresh mixture and combustion products in the direction from light to heavy fluid causes Rayleigh–Taylor instability. This diversity of the possible instabilities, despite numerous experimental data available (e.g., (Leyer, et al., 1971; Schadow, et al., 1992; Wu, et al., 2012), and considerable success in the understanding of the governing mechanisms (Oran, 2005; Searby, 1992; Bychkov, et al., 2006; Wu, et al., 2003; Wu, et al., 2009; Akkerman, et al., 2013; Bychkov, et al., 2002) of the instabilities, constitutes the origin of the status that only limited successes were achieved in the creation of the unified approach in flame instabilities modelling. Recent numerical simulations(Bauwens, et al., 2011; Yanez, et al., 2011; Molkov, et al., 2012), which take into account development of the instabilities, demonstrate that essentially successful approaches should be further generalized with the view to provide established methods for the engineering CFD simulations. In (Bauwens, et al., 2011) the simulation of the vented explosion introduces combustion model considering additional flame wrinkling which is described by a transport equation with the generation and removal of flame surface wrinkling. The relative simplicity and transparent physical basis of the method promise high potential for the use in applied simulations, however currently the method requires calibration which reduces the value from the standpoint of the immediate use of it. In (Yanez, et al., 2011), using numerical solution extending the theory of (Bychkov, 2002), study of the existence of spontaneous transition from the acoustic to the parametric instability and their growth rates were evaluated for a set of mixtures typical for hydrogen based applications. The accounting of acoustic instabilities was successfully utilized in benchmarking simulations (Kotchourko, et al., 2011), although some *backfitting* took place. A SGS combustion model of (Molkov, 2012), which uses the flame area growth equation based on fractal theory, provided reasonable agreement with experimental data down to ~12.8% H_2 concentrations, although requiring further development for other mixtures.

Combustion of the hydrogen-air mixtures was studied largely at standard environmental conditions, however new technologies often dictate substantial variation of the conditions which have to be taken into account for the safety analysis. Among others, the fundamental properties of hydrogen and hydrogen mixtures with other gases and dusts, including burnable and unburnable substances have to be considered. The amount of data on hydrogen behaviour at elevated up to 1000 bar and sub-atmospheric pressures, at elevated and lowered up to cryogenic temperatures, is very limited. Only few studies are available in the literature, e.g., sub-atmospheric laminar flame speeds (Kuznetsov, et al., 2011), combustion of the cryogenic jets (Friedrich, et al., 2011), combustion of the spills of the liquefied hydrogen (Statharas, et al., 2000; Hooker, et al., 2011).

IDENTIFICATION OF KNOWLEDGE GAPS

For the safety analysis an availability of experimental data, CFD models, and engineering correlations for the following issues can be qualified as having highest priorities:

- Explosions in real scale configurations in complex geometry with realistic obstacles and different level of confinement, including experimental data for the development of multi-phenomena combustion models for all flame acceleration mechanisms or mechanisms increasing mass burning rate.
- Flame acceleration and deflagration-to-detonation transition in a semi-confined to open geometries.
- Vent sizing methodology, including effect of vent cover inertia on vented deflagration dynamics
- Effect of obstruction characteristics on flame dynamics (acceleration/deceleration) and DDT for different confinement, including global and local quenching phenomena in different geometries and scales
- Experimental data and representative models for the unresolved small-scale obstructions affecting possible flame acceleration and DDT
- Effect of hydrogen concentration gradient on the possibility of on flame dynamics (acceleration/deceleration) and DDT for different confinement
- Flame instabilities (acoustic, parametric, Rayleigh–Taylor, Kelvin–Helmholtz, Richtmyer-Meshkov, Landau-Darrieus) and their effect on the flame dynamics including scaling conditions
- Partially premixed combustion, in particular triple flames in hydrogen-air layers and their pressure effects in confined space, including hydrogen jet combustion in confined and unconfined conditions
- Critical conditions for flame acceleration and DDT in cryogenic hydrogen-air mixtures
- Mechanisms of LH2 enrichment by oxygen and explosions after LH2 spills
- More experimental research is needed on laminar burning velocity for all ranges of pressure, temperature and equivalence ratio.

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7. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN HYDROGEN FIRES

EXECUTIVE SUMMARY

Hydrogen release might occur on storage, transport and handling. Credible storage methods include low and high pressure vessels, cooled liquid hydrogen tanks and solid hydrides. Leakages, broken fittings or connections as well as openings/holes formed by fragment impact or even the complete destruction of the storage could act as a possible source of hydrogen release. An ignition is likely for all forms of releases due to the wide range of flammability and low ignition energy (Astbury, et al., 2005; Dryer, et al., 2007; Mogi, et al., 2008). The type of storage or transport as well as the type of opening will guide the resulting fire. Released in containments, hydrogen would accumulate and mix up with air, the resulting mixture might deflagrate or even make a transition deflagration to detonation, DDT. The investigations use video/camera techniques, species sampling of the flame, temperature measurement and measurement of the emitted radiation. A pure hydrogen fire is nearly invisible (only weak water bands in the red spectral range), radiation is mainly emitted in the UV by OH-bands. Water bands cover the NIR and MIR spectral region. However, real hydrogen flames often include impurities or entrain them on propagation, resulting in addition of lines, bands and (Grey body) continua.

STATE OF THE ART

Fires from leakages to form laminar or turbulent diffusion flames

Releases from small leakages or small holes from hydride tanks generate normally a low momentum and ignition forms sustained laminar or turbulent diffusion flames. These are buoyancy driven and the main impacts of hot zones are vertically directed and might be considered also as jets. Detailed investigations occurred at laboratories to derive burning rates, species and temperature profiles. (Early standard work: Günther and Janisch (1972), and others later (Liu, et al.; Aung, et al., 1983; Parej, et al., 2010; Dahoe, 2005; Ilbas, et al., 2006). The results provided a basis for hydrogen combustion mechanisms (Warnatz, 1982; Peters, 2000; O'Conaire, et al., 2004; Li, et al., 2004), fire modelling and CFD simulation. The data on flame velocities depending on pressure are still limited to relative low pressures (< 3 MPa) (Iijima, et al., 1986; Kolarik, et al., 1991; Aung, et al., 1998; Bradley, et al., 2007), despite they are needed for fire and combustion studies. Emission spectroscopy has been successfully applied to small scale turbulent hydrogen diffusion flames (Gore, et al., 1987; Kounalakis, et al., 1988); and those under pressures up to 3 MPa (Kolarik, et al.; 1991), correlated to flame evolution. Simultaneous water vapour concentration and temperature measurements were performed in transient hydrogen flames (Blunck, et al., 2009). Flames (Schilling, et al., 1988; Pohsner, et al., 1994) were also studied in extremely high pressure environments up to 200 MPa applying UV-Vis emission spectroscopy with analysis of the OH-bands for temperature estimations with diatomic band evaluation method (see Schneider, et al., 1988; Eckl, et al., 1992). Still the detection and identification of small hydrogen releases and beginning fires is difficult (Greco, et al., 2011; Buttner, et al., 2011; Linke, et al., 2011; Cleary, et al.; 2011).

Jet fires produced from openings/holes in storage containers or broken fittings or connections

Momentum driven jet fires are generated on openings of high pressure storage tanks or liquid tanks, or fuel cells by holes at ambient temperatures. These jets might impose materials or humans a the distances up to 15 m, depending on the release conditions, mainly vessel pressure, mass flow rate and momentum. The hydrogen jet head propagates at high velocities entraining air in a turbulent way. During such hydrogen releases, an early ignition of the flammable hydrogen air mixture is more likely to develop into a fire (Ruban, et al., 2011; Chang Jong, et al., 2011;

Wen,) or a jet-fire (Astbury, et al., 2055; Dryer, et al., 2007; Mogi, et al., 2008; Veser, et al., 2009; Mogi, et al., 2008; Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011) depending on the impetus. However, hydrogen might also accumulate (especially in confined volumes) and initiate premixed deflagration producing high overpressures or a DDT. Even more hazardous are under-expanded jets which may increase in size and keep higher temperatures, downstream.

Research tries to measure the size (length and width) of the fire, the radiative properties depending on the initial pressure in the tank and the opening diameter or study the effect of barriers on the fires (Molkov, 2012; Kalghatgi, 1984; Ruffin, et. al, 1996; Shevyakov, et al., 2004; Shirvill, et. al., 2005; Schefer, et. al., 2007; Imamura, et al.; 2008; Mogi, et al., 2009; Proust, et al., 2009; Studer, et al., 2009; Veser et al., 2009; Saffers, et al., 2011; Houf, et al., 2007; Houf, et al., 2008; Deimling, et al., 2011; Grune, et al,. 2009; Gavrikov, et al,. 2009; Grune, et al.,. 2011).

Hydrogen jets form a cone the half angle of which is between 8 and 12° independent of the orifice diameter, an angle which is generally found for jets or even for rocket plumes or expelled powders which propagate at various velocities. The resulting hydrogen jet might ignite and establish a sustained turbulent flame. This process consists of 2 steps, a highly transient one, starting from the point of ignition propagating simultaneously downstream and upstream the jet; followed by the flame pulsating till its stabilization. As the turbulent hydrogen jet has already entrained air the first phase can develop as a gas explosion/deflagration beginning from the point of ignition, upstream and downstream. For high initial mass flow rates (> 400 g/s) the apparent flame velocities might approach near sonic speeds and generate substantial pressure waves (see visualization by BOS-method of Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011). The molecular band modelling code BAM from Fraunhofer ICT (details see Weiser, et al., 2005, various application since 1994 are in Eckl, et al., 1995; Deimling, et al., 1997) enabled the time resolved evaluation of the species concentrations and temperatures using robust fast scanning IR-Spectrometer (Blanc, et al., 2009; Blanc, et al., 1988). Temperatures found are close up to 2000 K with transient zones up to 2400 K (Veser, et al., 2009; Mogi, et al., 2008). The results of Houf and Shefer (2007) are obtained using the RADCAL code (Grosshandler, et al., 1993). It is interesting that the strong CO_2 band from entrained air can be used to estimate the air content (Blanc, et al., 2009; Blanc, et al., 1988).

Highly transient jets which are built up from bursts of high pressure storage tanks and from liquid hydrogen tanks can induce also auto-ignition. Negative Joule-Thomson effect might combine with reflected shock waves from obstacles originally generated by the burst might to enable initiation. The exhaust from an opened liquid hydrogen tank (Pehr, 1996) trigger pulsating with subsequent overlapping transient jets lasting several seconds, which can be connected with partial exhaust blocking by the initiated deflagration of the jets (Eckl, et al., 1995). Generated pressure waves were moderate in the kPa range (Pehr, 1996; Eckl, et al., 1995). Temperatures were found in (Eckl, et al., 1995) to be similar to those of sustained turbulent jets up to 2000 K with some hot spots up to 2400 K (Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011; Eckl, et al., 1995). Recent work (Friedrich, et al., 2011) concerned quasi-stationary jets from liquid reservoirs. Sound levels and radiation were measured and are related to various flow parameters and release phases. Note, that the radiation measurement is not adequate to get reliable quantitative results, however they are used to estimate flashback scenario and scaling.

Jet fires are well studied under laboratory conditions at small scale. Profiles including air entrainment are well understood. Nonetheless at larger scale the deviations can take place. It was shown, that the air entrainment can be obtained by fast IR-spectroscopy analysing the strong CO_2 band (wavelength 4.25 μm) from the involved air (Blanc, et al., 2009; Blanc, et al., 1988). It would be wise to apply imaging spectroscopy resolving fluctuations to the jet fires to get a full spectral picture of the jet in comparison to the video analysis. Realistic integrated radiation can be derived by this approach and simulated by obtaining temperature and species distributions over the jet fire applying codes like RADCAL (Grosshandler, 1993) or the BAM code (Weiser, et al., 2005; Blanc, et al., 2009; Blanc, et al., 1988).

For visualization the BOS-technique (Keßler, et al., 2005;) should be applied which has been adopted by some research groups (Veser, et al., 2009; Mogi, et al., 2008), however improvements (see later) could be combined with brightness subtraction (Otsuka, 2007) or one-dimensional frame compacting the latter provides transient flame profiles (Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011).

The use of barrier and wall for preventing jet impingement has to be carefully planned (Houf, et al., 2009; Willoughby, et al., 2009).

Transient fires have been investigated experimentally at already large scale years ago in open air. Explosions premixed hydrogen air clouds, mainly were ignited in symmetric configurations of balloons or in long plastic tubes to investigate apparent flame velocities depending. This velocity increases with cloud size (Pförtner, 1983; Makeev, et al., 1983; Molkov, et al., 2005; Tang, et al., 2009) or tube length (Ciccarelli, et al., 2008). Obstacles, lattices enhance it too. An overview on the dependence of the burning rate on various parameters is given by Dorofeev (1995, 1995, 2005, 2000), the resulting pressures reach up to some tens of kPa. The fireball from a gas explosion is substantially larger than the initial ignited mixture given by the expansion ratio. In addition, this fire ball sustains, moves (mainly upwards, if no wind) and cools down, still substantially radiating also for fast transient fires. A DDT was predicted to occur (Lee, 1977) and verified in various sizes (Pförtner, 1985; Dorofeev, et al., 2001) which might be induced by flame enhancement of turbulent flow fields. It deploys a cell structure. A SWACER effect was also postulated (Lee). Accumulated gas in containments leads to an increasing pressure due to the expansion factor of the oxidation which might lead to failure of the containment structures, the walls of which getting strong acceleration. A Gurney – Energy relation might be a valid approach to describe the fragment velocities.

Release and fires of hydrogen in closed containments leads to explosions with rising pressure (Pitts, et al., 2011). Starting from experiments in closed vessel which mainly gave apparent flame velocities to derive laminar flame velocities (Iijima, et al., 2005; Milton, et al., 1984; Kolarik, et al., 1991; Jo, et al., 2010). Numerical calculation already by Warnatz (1981) correlated well with experimental values. Spectroscopic results can be correlated to flames at ambient pressures when considering species concentrations (water). Fast scanning NIR spectroscopy (e. g. AOTF-spectrometer (Ludwig, et al., 1973; Ferriso, et al., 1965; Kneizys, et al. 1996) with scan rates up to 1.5 μm/ms) can more or less observe the strongest intensities of the emitted radiation from hydrogen-air explosions resolved in time. The combined effects for example of stoichiometry and pressure (Bradley, et al., 2007; Kuznetsov, et al., 2011) or turbulence and pressure (Kobayashi, et al., 1996), the influence of external turbulence is not yet fully investigated.

Metal hydrides

Metal hydrides (Züttel, 2003) exhibit high potential to meet the US DOE (Programm Review 2004) system targets for automotive hydrogen storage. Recent material development and basic hydride research has led to significant improvements in the metal hydride properties (thermodynamics and kinetics). Early developments use heavy metal hydride which operates under moderate pressures. The hydrogen release is of moderate speed due to the fact that it is endothermal and is controlled by diffusion. This is also true for light metal hydrides. The hazards will rise, however, if, in addition, the unpassivated light metals can get access to air, since the nano-structured metal is immediately oxidized (Weiser, et al., 2007; Eisenreich, et al., 2011) strongly heating the storage device. A destruction of the storage containers might be expected generating a highly pyrophoric cloud in hydrogen (Lohstroh, et al., 2007; Anton, et al., 2007; Tanaka, et al., 2009; James, et al., 2009; Dedrick, et al., 2009).

Contours and radiation from hydrogen fires

Currently, high speed video techniques have mainly been applied to record the shapes of emitting fires, where shapes of flames are usually recorded by seeding tracing material into the flame. In technical flames, these are sodium or soot as "dye" from impurities for the "invisible" hydrogen fires. *Schlieren* techniques can make the structures of the flames visible (Raffel, et al., 2000). The BOS, background oriented *Schlieren* technique, can not only visualize the shapes of hydrogen fires, but also can reveal detailed structures and additionally can provide statistical data of turbulence (Veser, et al., 2009; Mogi, et al., 2008; Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011; Blanc, et al., 2009; Blanc, et al., 1988; Keßler, et al., 2005; Kotchourko, N., et al., 2011). Although the obtained images are impressive, the question how they can be correlated to flame structures and simulation results remains open; an example of further development the technique similar to the *Schlieren* is discussed in (Pitts, et al., 2011). A comparison with detailed imaging spectroscopy and CFD simulation could outline the correlation to real turbulent effects. In addition, blast waves can be made visible (Deimling, et al., 2011; Grune, et al., 2009; Gavrikov, et al., 2009; Grune, et al., 2011). The combination with brightness subtraction methods (Friedrich et al., 2011) might help to clarify the meaning of the structures.

Beneath of direct contact with the flame jet or fire ball, radiation from hydrogen fires is another important stand-off effect. The radiation intensity depends on species, duration in the hot zones existence and the temperature distribution. Radiation is mainly seen as a passive effect for remote sensing and the endangering of the hydrogen fire variants. Whereas in laboratory experiment all types of modern spectroscopic methods (UV-Vis-IR-, Raman Spectroscopy, CARS, LIF, PLIV, etc.) were applied, for large scale hydrogen fires robust emission spectroscopic methods have to be preferred. Hydrogen fires are band emitters with temperatures reaching to 2500 K, predominantly those of OH in the UV-spectral range (band maximum 309 nm) and H_2O in the NIR and IR spectral range (various bands in the wavelength range from 0.640 - 9 μm with varying emissivity of band maxima. The effective emitting surface has a different distance to the spectrometer for each band). The different bands approach the intensity of a Black Body radiator at the band maximum wavelength for large fires (Weiser, et al., 2005), therefore commonly used pyrometers are not applicable. CO_2 is entrained by air and can be identified because of the strong band at 4.25 μm, which can be used to measure the air entrainment (Blanc, et al., 2009; Blanc, et al., 1988). Impurities contribute single atomic lines (Na, K, Li, Ca, Fe etc.) and continua (mainly soot from organic contaminants) (Eckl, et al., 1995). If turbulent structure in jets have to be measured or transient phenomena like gas explosions, then fast scanning spectrometers should be used. Such robust systems for the NIR-IR spectral range are, for example, filter wheel spectrometer with continuously varying spectral transparency with rotating angle with scan rates up to some 100 spectra/s and produce complete spectra or AOTF (acousto-optical tuneable filter) spectrometer with scan rates up to 1.5 μm/s (Kolarik, et al., 1991; Weiser, et al., 2005; Blanc, et al., 1988). Both types can be upgraded to imaging spectrometer by using (CCD) camera detectors. They were extensively used for investigation of transient fires like pulsating pool fires, pyrotechnics, propellant flames, rocket plumes, gas explosions, solids/dust explosion, etc. Currently, robust FTIR-spectrometers are available for fast scanning and imaging spectroscopy which provide higher wavelength resolution. To study the OH-band in the UV there have been already OMAs (Optical Multi-Channel Analyzer) used for more than 30 year with time resolution of 10 ms and more (Kolarik, et al., 1991; Schneider, et al., 1988; Eckl, et al., 1992; Weiser, et al., 2005).

The evaluation of the 3-atomic molecules uses the "Handbook Infrared Spectra of Hot Gases" which gave the basis of Hitran, Modtran and Lowtran- code series of the NASA (Ferriso, et al., 1965; Kneizys, et al., 1996). These codes were made applicable for every-day use by the codes RADCAL (Grosshandler, 1993) of Grosshandler and the BAM-code of Fraunhofer ICT (Weiser and Eisenreich, 2005). RADCAL is a simulation code whereas BAM is, in addition, able to perform a least squares fit procedure of spectral data resulting in species and temperature distributions of the radiating source (including also Grey Body soot emission) and has been applied in numerous cases (see e.g. Weiser, et al., 2005; Eckl, et al., 1995; Deimling, et al., 1997; Blanc, et al., 2009; Blanc, et al., 1988).

The radiation emitted from the fire ball which contains OH radicals and other molecules which play important roles in the reaction mechanism (Warnatz, et al., 1982; Peters, 2000; O'Conaire, et al., 2004; Li, et al., 2004) like H_2O_2 (see e.g. Johnson, et al., 2009) and HO_2. The reaction fronts being exposed to the intensive radiation and might therefore modify the reaction mechanism used in combustion modelling. It might occur that the radiation emitted from the fire ball interacting with flame front species can contribute also substantially to the increase of burning velocity depending on the size of hydrogen-air mixtures in comparison without accounting of this effect. Including chemical kinetics into CFD modelling might contribute to an improved understanding of DDT (Liberman, et al., 2011).

Long term aim (a really challenging task) can be expressed as follows: joint research to combine transient shapes, structures and spectroscopy resolved time and space of hydrogen fires with CFD modelling, which includes full reaction kinetics and radiation transport of key molecules of reaction mechanisms.

IDENTIFICATION OF KNOWLEDGE GAPS

- For large scale jet fires, there exists only limited number of methods to investigate, whereas the conditions forming jets can vary in a broad range, including different initial pressures, temperatures, hydrogen mass flows and the environmental conditions, such as obstacles and barriers.
- At the initial stage of a jet fire (just before the non-premixed turbulent flame is established), due to the existence of the partially premixed cloud, hypothetically fast premixed flames (so-called "delayed ignition" deflagration) and DDT event cannot be excluded, therefore critical conditions necessary for the hazardous jet fire dynamics have to be identified.
- For the obtaining the realistic integrated radiation for large scale fires it looks rational to apply imaging spectroscopy resolving fluctuations to the jet fires to get a full spectral picture of the jet in comparison to the video analysis.
- The results of the BOS-technique should be validated in comparison with numerical simulations. Use BOS–measurements with not expensive video cameras for detection and identification of effects induced.
- Currently there is little experimental data available for the transient pulsating jet fires from liquid hydrogen or tanks at high pressures.
- Jet fires in containments should be studied in more detail. Improvement of early detection of leakages and related fires, especially important in containments.
- Basic investigations of effect of small scale hydrogen fires (microflames) on materials
- Radiation effects at various distances, including CFD and engineering methods.
- Simulation of fireballs, their cooling down and movement dynamics, especially for large clouds, where cooling occurs mainly by radiation.
- Investigation of explosions in containments and acceleration of fragments depending on the durability of containments
- Investigation of the hydrogen release from various types of currently favoured hydrogen storage materials and the effects of real storage containers, depending on loading status, operational state, ambient temperature etc.
- Investigation of accident/crash situation including hydride storage facilities.

- Apply fast scanning spectroscopy to fires and evaluate species concentrations and temperatures by least squares fit procedures, preferable would be imaging spectroscopy also to clearly visualize the reacted areas (fireballs) in contrast to the reaction zones.
- Study of large scale hydrogen fires of all types mentioned above to get reliable models of radiation of large hydrogen fires which include interaction of radiation with reaction species of the reaction front.
- Extend BOS techniques by synchronized 2 cameras, further develop 3D BOS video analysis by comparison with CFD simulation to evaluate the meaning of the observed structures. Correlate 3D BOS with radiation shapes and CFD modelling which includes radiation transport.
- Parametric studies of indoor fire behaviour, including phenomena of self-extinction, external flame and re-ignition.

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8. RESEARCH STATE OF THE ART AND KNOWLEDGE GAPS IN ENGINEERING CORRELATION SCIENCE

One of the key tasks of scientific work is to translate fundamental scientific findings into practical formulas, which are easily applied in daily work. In many cases financial or computational resources and - even more often - time is limited, such that a physically resolved numerical solution of the complex phenomena relevant for hydrogen safety issues is practically impossible. Although CFD solvers and computer performance are developed further continuously, validated simplified correlations often suffice for first estimates or sensitivity studies with a large number of varying parameter settings.

So, the simplified toolset consists of all kind of empirical correlations, criteria, statistics and models based on first principles, which are needed to assess the risk implied with certain hydrogen inventories or fluxes in user defined scenarios.

Such a toolset shall be based on robust, published, state-of-the-art correlations. The design shall be highly modular and fast response times of the system are necessary to make it different from the more complex tools like CFD.

The tools shall be maintained by the hydrogen safety research community itself. As safety is a public concern and a big part of relevant scientific work is funded by public agencies anyhow, the toolset should be an open and free software system, which is well documented and quality assured in a cooperative manner. Potential adopters of this work might be the HySafe association or the safety task of the IEA HIA.

Each tool of the toolset shall consist of a set of input parameters and a set of output or result parameters. The model calculates the output with the actual input. Each engineering method must have a clear range and conditions of its applicability. All input and output parameters are elements of the respective scenario. Each tool shall be described in detail, the valid range of input parameters has to be controlled appropriately, literature references should be given and model tests have to be provided.

A typical use case will consist of a user defining explicitly a new scenario by giving the inventory or hydrogen flow rate, geometrical settings like confinement and/or congestion, mitigation measures, up to a leak size, etc. For a statistical analysis any of these scenario properties might be defined by a probability distribution instead when applicable. Then he might choose a tool to act on the scenario. The input, which was not yet defined but required by the selected tool, shall be input by the associated tool interface. If any of the input parameter lies outside the models validity range an appropriate action shall be taken. Appropriate measure is warnings or even an exception. Any output defined before the execution of the model, shall be overridden by the model. A warning will be issued.

Users with appropriate rights may edit tools or define new tools. New tools might use existing ones by calling them in a specific sequence or even recursion should be possible. These kinds of models shall be called "super-models". An example for such a super-model could be the tool for calculating flame radiation which would rely typically on the determination of a Froude number, suitable models for flame length and width, residence time, radiant fraction and so on.

With all requirements defined so far a WEB2.0 technology kind of implementation is envisaged. A system which allows for immediate testing and on-the-fly editing of the tools is the Smalltalk dialect Squeak based dynamic web development framework Seaside.

9. CONCLUSIONS AND RECOMMENDATIONS

Below is the list of only some of deterministic knowledge and technological gaps in hydrogen safety. They are waiting to be closed to underpin emerging technology by firm hydrogen safety engineering design without compromising life safety and property protection, i.e. public acceptance. The main gap in QRA is quantification of probabilities of various events that represents everlasting question and dispute that will be probably resolved when statistics of system failure in real use by public (not by professionals) will be gathered. More deterministic studies should be performed to close numerous knowledge gaps and statistics of hydrogen system failure modes gathered before the risk assessment methods, that are developed well theoretically, can be applied with reasonably uncertainties.

Thus, the focus of hydrogen safety research currently should be today on the development of innovative engineering solutions and breakthrough safety strategies, e.g. to design and manufacture a high-pressure storage tank (type 4) with fire resistance up to 2 hours to allow release with flame length below 1 m for hours to allow self-evacuation and rescue at accident scene.

The list of knowledge and technological gaps in hydrogen safety and relevant actions include but not limited to:

- Fire resistance rating (standing in fire without losing integrity either by leak or shell rupture) of storage tanks has to be increased drastically to provide life safety and property protection through design, manufacturing, and testing of new generation of tanks. Requirements to fire resistance rating of hydrogen systems, including their matching to fire resistance rating of structures and buildings.
- Safety at refuelling stations is often out of hands of professionals that gives examples of using 20 mm pipes from 700 bar storage to dispenser (kind of WMD in case of full bore rupture). This has to be tackled either through enforced education of designers or subcontracting hydrogen safety experts.
- Existing methods for calculation of safety distances for liquid hydrogen are based on data obtained in early 1960's - 1970's. Those correlations did not anticipate such significant amounts and as such cannot be used for reliable calculations. New correlations are needed for describing:
    - Spillage of large quantity of LH_2 on ground or seawater
    - Cloud dispersion of cold hydrogen from vent and its ignition
    - Performance of various thermal insulation options
    - Safety distance as function of LH_2 quantity and re-assessment of the scientific basis for existing correlations
    - Evaluation of related hazards and their consequences
- Correlations for attached jets, especially for an extent of a flammable envelop.
- An overpressure of a delayed ignition deflagration of a jet flammable envelope.
- Simulation of fireballs, their cooling down and movement dynamics, especially for large clouds, where cooling occurs mainly by radiation, along with tank rupture and blast wave decay.
- Simple for use tools for hydrogen safety engineering. As safety is a public concern and a big part of relevant scientific work is funded by public agencies anyhow, the toolset should be an open and free software system, which is well documented and quality assured in a cooperative manner. Potential adopters of this work might be the HySafe association or the safety task of the IEA HIA.
- Releases and dispersion of liquid hydrogen indoors and requirements to ventilation systems

- Prevention and mitigation of destructive overpressures enhanced by interaction of combustion with enclosure walls (acoustic flame instability) during vented deflagrations of lean hydrogen-air mixtures.
- Specificity of flashover and backdraft phenomena for fires including hydrogen systems
- Extinction of hydrogen jet fires indoors and outdoors, including tactics for firemen intervention
- Education and training programmes have to ensure that new knowledge and the progress in inherently safer use of hydrogen and fuel cells reaches as much developers as possible. New education/training activities should be established in hydrogen safety involving all stakeholders, especially for experts responsible for safety in projects, e.g. funded by European FCH JU. This education activity would provide a means to equip the human capital, who will drive the development of inherently safer hydrogen systems and infrastructure forward. This could be done e.g. through a funding of a pan-European education programme within cross-cutting activities of FCH JU.

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Abstract

Wide spread deployment and use of hydrogen and fuel cell technologies can occur only if hydrogen safety issues have been addressed in order to ensure that hydrogen fuel presents the same or lower level of hazards and associated risk compared to conventional fuel technologies. To achieve this goal, hydrogen safety research should be directed to address the remaining knowledge gaps using risk-informed approaches to develop engineering solutions and Regulation Codes and Standards (RCS) requirements that meet individual and societal risk acceptance criteria, yet are cost-effective and market-competitive.

IA HySafe and JRC IET partnered to organize a Research Priorities Workshop in Berlin on October 16-17, 2012 hosted by BAM (on behalf of IA HySafe) to address knowledge gaps in CFD modelling of hydrogen safety issues. The findings of the workshop are described in the report. The document aims to become a reference document for researchers/scientists and technical (including industry) experts working in the area worldwide. It is also a welcomed contribution for the Fuel Cell and Hydrogen Joint Undertaking (FCH JU) and for other funding bodies/organizations that must make decisions on research programmes and during the selection/choice of projects to be financially supported pursuing the safe use of hydrogen within Horizon 2020 framework.

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