Scientific Principles of e-Laboratory of Hydrogen Safety

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ABSTRACT

Education and training are crucial for provision of safety of fuel cell and hydrogen (FCH) systems and infrastructure. The European project "Novel Education and Training Tools based on digital Applications related to Hydrogen and Fuel Cell Technology" (NET-Tools) is developing digital platform and providing online contemporary tools and information services for education and training within FCH sector. The project is delivering an innovative platform, influencing robust and effective learning while offering a unique blend of novel digital tools. The platform has two main pillars, i.e. e-Education and e-Laboratory. The essential part of e-Laboratory is a suit of hydrogen safety tools. The aim of this paper is to present scientific principles behind the hydrogen safety engineering tools of the e-Laboratory. The principles describe or predict a range of natural phenomena in unignited releases, jet-fires, deflagrations, blast-waves and fireball etc. They summarize and explain a large collection of facts determined by experiments and supported by physics and mathematics. Principles are tested based on their ability to predict the results of future experiments and possible safety related scenarios to calculate flame lengths, concentrations, overpressures, hazard distances, etc., and supported by peer-reviewed publications.

KEYWORDS: Deflagration, ventilation, jet fire, blast wave, fireball.

INTRODUCTION

Education and training for emerging fuel cell and hydrogen (FCH) sector is critical for professional development of current and future workforce. This underpins the leadership and competitiveness of European FCH products. The European project "Novel Education and Training Tools based on digital Applications related to Hydrogen and Fuel Cell Technology" (NET-Tools) is developing digital infrastructure and providing contemporary online tools and information services for education and training within FCH technologies sector.

The NET-Tools project is delivering a technology platform, influencing robust and effective open source and free access learning management system while offering a unique blend of novel digital tools encompassing generic information, education and research. The digital platform includes two main pillars i.e. e-Education and e-Laboratory. The platform addresses educational interests of various groups of stakeholders with different levels of education from higher schools and universities, both undergraduate and graduate students, to professionals and engineers from industry, offering both e-learning modules and on-line design tools. The aim of this paper is to give an overview of the scientific principles that lay behind the engineering tools developed within Safety Engineering Toolbox of e-Laboratory.

Performance-based calculation of hazard distances, the term introduced recently by ISO TC197 Hydrogen Technologies, is a key element of hydrogen safety engineering of FCH systems and infrastructure, e.g. refuelling stations. The principles behind the e-Laboratory of Hydrogen Safety allow assessing hazard distances for unignited releases (flammable envelope size); ignited releases

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(jet fires); blast wave decay from deflagrations, detonations and high-pressure hydrogen storage tank rupture in a fire, fireballs, etc. This long expected by hydrogen industry toolbox provides determination of hazard distances for unignited releases and jet fires in interactive regime, e.g. by varying system parameters like pressure and pipe (leak) diameter. The state-of-the-art safety tools of the e-Laboratory of Hydrogen Safety is a free-access expanded European analogy of the HyRAM (Hydrogen Risk Assessment Methods) tool, which has been developed by Sandia National Laboratories (SNL) during last decade under funding of the US Department of Energy. The e-Laboratory demonstrates European leadership in hydrogen safety engineering, e.g. by capability to calculate hazard distances determined by thermal and pressure effects from a fireball and blast wave after tank rupture in a fire, which are absent in the HyRAM tool and similar Canadian (UTRQ) framework is implemented using Smalltalk Seaside web development environment.

SCIENTIFIC PRINCIPLES

This section describes scientific principles behind the engineering tools of the e-Laboratory of Hydrogen Safety. The tools are gathered in groups by similarity in applications.

Unignited releases

The under-expanded jet theory [1], [2] is behind the "Jet parameters" and other tools related to under-expanded jets. It allows calculation of hydrogen flow parameters in real and notional nozzles. Density in the real nozzle is needed for the use in the similarity law for concentration decay in hydrogen jet [2], [3] and parameters at the notional nozzle, which are widely used as boundary conditions for computational fluid dynamics (CFD) simulations. The tool allows calculation of mass flow rate of high-pressure hydrogen release through both a hole in a storage vessel and a narrow channel with losses. The tool for prediction of axial concentration decay of a leaking hydrogen for sub-sonic, sonic, and super-sonic jets employs the similarity law, which is validated in a wide range of conditions from expanded to highly under-expanded jets [2]. This tool calculates hazard distance, i.e. length of the flammable envelope, for momentum-dominated jets, which represent practically all realistic releases from high-pressure hydrogen equipment and storage.

The under-expanded jet theory is used to build and validate described in the next section the universal similarity law, which is valid for both expanded and under-expanded jets in the momentum-controlled regime. The theory is applied to derive: the universal correlation for hydrogen jet flame length, the tool for calculation of blow down time of hydrogen release from the storage vessel, etc. The theory is essential to carry out hydrogen safety engineering for different applications.

The similarity law

It must be noted that thermal effects of jet fires, pressure effects of deflagration or detonation, and pressure and thermal effects of high-pressure storage rupture in a fire (blast wave and fireball) could override the hazard distance determined by the size of flammable envelope or hazard distances of a jet fire. Thus, knowledge of laws describing hydrogen dispersion and flammable cloud formation, including axial concentration decay for arbitrary jets is essential for hydrogen safety engineering.

Figure 1 shows the similarity law for prediction of axial concentration decay of a leaking gas for sub-sonic, sonic, and super-sonic jets is derived and presented in [2], [3]. It is valid in a wide range of conditions from expanded to highly under-expanded jets. It can be applied for calculation of hazard distances informed by the size of the flammable envelope. The non-ideal behaviour of hydrogen at high pressures and the under-expansion of flow in a nozzle exit are considered by employing the Abel-Noble equation of state (EoS) for real gas.

It can be seen that all experimental points are on or below the similarity law line. This is thought due to friction and minor losses in experimental equipment, which were not accounted for when the under-expanded jet theory without losses was applied. Indeed, from the similarity law equation it follows that if losses decrease pressure at the nozzle exit, and then they reduce hydrogen density and therefore the concentration in the jet for a fixed distance from the nozzle. This is equivalent to shifting experimental points down on the graph. If the spouting pressure (actual nozzle exit pressure) is applied instead of the pressure in a storage tank the difference between the similarity law curve and experimental data would reduce to zero in the limit. The universal character of the similarity law for both expanded and under-expanded jets makes it an efficient tool for hydrogen safety engineering.

For hydrogen jets into stagnant air for a fixed concentration expressed in percent by mass C_{ax}, the ratio of a distance, x, to the nozzle diameter is a constant, i.e. x/D=const. This means that the distance to the lower flammability limit (hazard distance) is directly proportional to the leak diameter. Thus, the design of hydrogen and fuel cell systems has to be carried out bearing in mind the requirement to minimise the internal diameter of piping, i.e. leak size for conservative full bore rupture scenario, yet keeping technological requirements to mass flow rate.

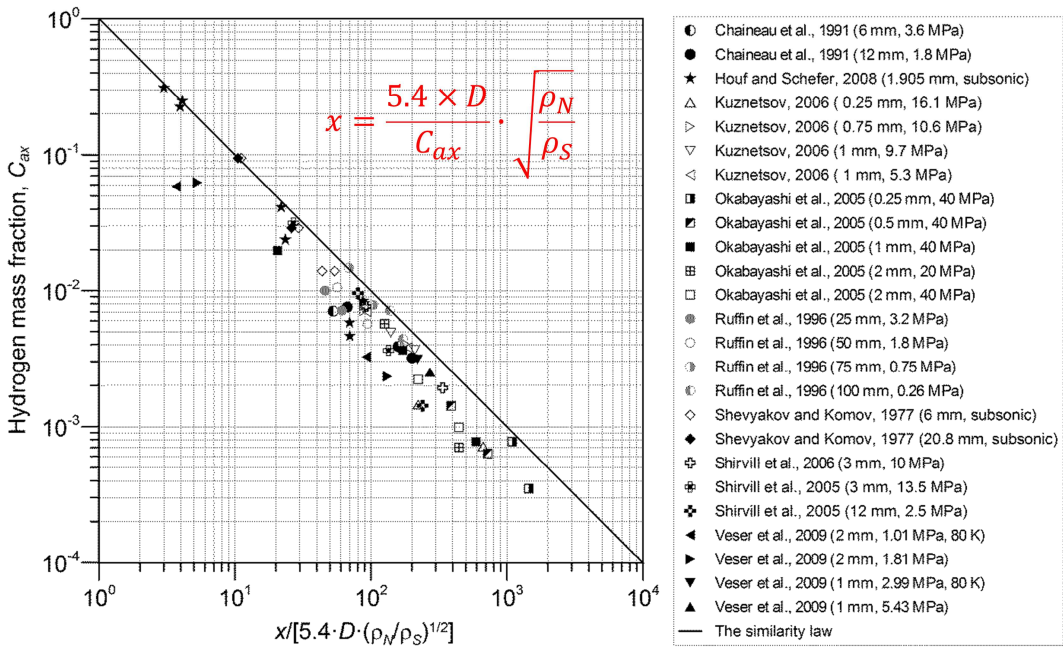

Fig. 1. Similarity law [2].

Effect of buoyancy

The "Effect of buoyancy" tool allows to calculate the decrease of hazard distance for initially momentum-dominated hydrogen jets when it transforms to buoyancy-controlled jet. It is based on validated against experiments the theory of Shevyakov which can be found elsewhere [2]. The engineering technique [2] qualifies which part of hydrogen jet (both expanded and under-expanded) is momentum-controlled with the rest of the jet downstream being buoyancy-controlled.

There are three types of jets depending on the role of buoyancy Fig. 2 (left): fully momentum-controlled jets are not affected by buoyancy; fully buoyancy-controlled jets are quickly diverted from the horizontal to vertical flow direction; the third type of jets is transitional with momentum-dominated part closer to the nozzle and buoyancy-controlled flow further downstream when the jet velocity drops and diameter increases. For hydrogen safety engineering it is important to know when this transition takes place. This has direct implication on hazard distance and thus the infrastructure cost.

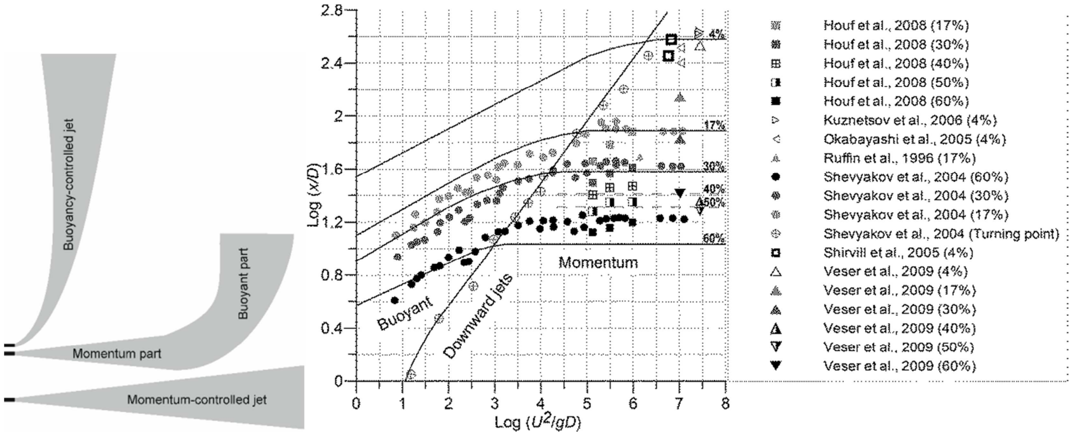

Fig. 2. Types of jets depending on the role of buoyancy (left), dependence of the distance to the nozzle diameter ratio *x/D,* for particular hydrogen concentration in air, on the Froude number (right).

Five theoretical curves (solid lines) and experimental data for expanded jets, and data of other researchers for under-expanded jets are shown in Fig. 2 (right). Practically all under-expanded jets in hydrogen incidents/accidents will be in the momentum-controlled regime as follows from available tests applied to validate the correlation. Four of five theoretical curves in the graph are related to hydrogen concentrations of 4%, 17%, 30%, and 60% by volume respectively. Each of these four curves has an ascending buoyant part and a momentum "plateau" part. The fifth curve "Downward jets" is of special interest. It gives for a jet directed vertically downward a dimensionless distance from the nozzle to the turning point, where the jet changes direction of flow from downward to upward. The fifth curve intersects each of the four other curves in the graph in the region of transition from momentum-dominated to buoyancy-controlled flow as expected.

The following sequence is applied in use of the correlation in Fig. 2. Firstly, the nozzle exit Froude number is calculated and its logarithm. The under-expanded theory is applied to calculate the notional nozzle exit diameter and the velocity in the notional nozzle exit when applicable. Then, a vertical line is drawn upward from a point on the abscissa axis equal to the calculated Froude number logarithm. The intersection of this vertical line with the line marked "Downward jets" on the graph indicates the concentration above which the jet is momentum-dominated and below which the jet is buoyancy-controlled and logarithm of the distance to the nozzle diameter. Further intersection with theoretical curves gives the distance to concentration of interest where the jet is buoyant by potentiation of *log(x/D)*. The idea behind the engineering tool lays in representation of the curves by the set of polynomial functions of the curves and the sequence of logical expressions to solve the problem.

The easy to apply technique Fig. 2 (right) can be very useful to develop cost-effective hydrogen safety engineering solutions. For instance, hazard distance for a horizontal jet release can be essentially reduced as only the length of the momentum-dominated part of the jet can be taken as an indication of the separation rather than the aggregated distance, i.e. both momentum- and buoyancy-controlled parts of the jet to the lower flammability limit (LFL) of 4% by volume of hydrogen.

Blowdown

The "Blowdown of storage tank" tool calculates pressure dynamics inside the tank during release for adiabatic and isothermal conditions, which can be combined to reproduce blowdown dynamics closer to reality. Both models give close pressure dynamics but different temperature dynamics of the released hydrogen.

The adiabatic blowdown model is based on the assumption of a quick release from a high-pressure reservoir and negligible heat transfer effects to the released hydrogen temperature. The adiabatic model gives lower temperature of released hydrogen at the end of the process. While, the isothermal blowdown of a storage tank assumes of a relatively long release from a high-pressure reservoir, so that heat transfer significantly changes the temperature of the outflowing hydrogen. The combination of adiabatic at the beginning and then isothermal model afterwards gives a good approximation for dynamics of temperature of released hydrogen observed in experiments.

Both models are built on the model for expanded and under-expanded jet parameters, which describes parameters in an expanded and under-expanded jet through the characteristic stages of its development – in the storage reservoir, the orifice, and the notional (effective) nozzle exit and utilises Abel-Noble EoS and the conservation equations for mass and energy.

The tool can be used to formulate mitigating measures and safety strategies based on fire resistance rating of onboard hydrogen storage tank. The fire resistance rating should be greater than the sum of time for a thermally activated pressure relief devices (TPRD) initiation and blowdown time of the storage tank to exclude its catastrophic failure in the case of fire. Obviously, the use of a TPRD with a larger diameter would create a larger flammable cloud or a jet flame. It would generate higher overpressure during "delayed ignition" or deflagration of turbulent flammable cloud. By this reasoning the TPRD diameter should be reduced as much as possible provided the fire resistance rating is increased consequently.

Passive ventilation

The "Passive ventilation" tool allows to calculate hydrogen concentration in an enclosure with known vent size for the given release rate or solve inverse problem method (calculate vent size to keep concentration below desirable level for known hydrogen release rate).

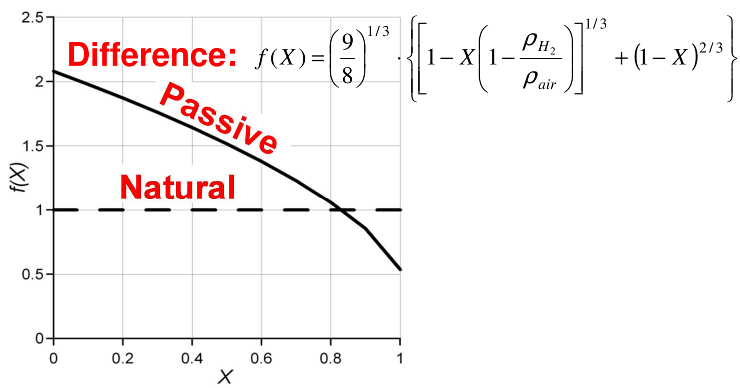

Fig. 3. Difference between passive and natural ventilation.

The model is developed in the assumption of perfect mixing and equations for passive (release of flammable or toxic gas) and natural (air quality problems) ventilation were compared [4] to show the essential difference between two approaches. The natural ventilation equations are usually derived in the assumption that the neutral plane is located at the half of the vent height, however for the passive ventilation of accidental release in an enclosure the neutral plane can be located anywhere below the half of the vent height. The development of passive ventilation model has demonstrated that the accurate analytical solution for passive ventilation differs from the approximate solution for natural ventilation by more than 2 times for lean and rich mixtures as shown in Fig. 3, where X is hydrogen mole fraction.

This could have serious safety implications and should be dealt with care while performing safety engineering involving hydrogen releases. The passive ventilation theory states that, vertical vent is more efficient compared to horizontal vent of the same area and this should be taken into account during the design of passive ventilation systems.

Forced ventilation

The "Forced ventilation" tool calculates parameters of the mechanical ventilation system to keep hydrogen concentration below required level. The parameters include the volume flow rate of air required for the given mass flow rate of hydrogen to be lower that specified limit in the assumption of perfect mixing. The model is based on the principles of passive ventilation and its calculation of ventilation flow rate to provide hydrogen concentration in an enclosure below required level. Application of forced ventilation in numerical experiments proved calculations and demonstrated a decreased gas concentration to the required level. This confirms that the proposed methodology can be applied to calculate the ventilation rate for fuel cell and hydrogen systems and can be used as a tool for hydrogen safety engineering.

Pressure peaking phenomenon

The revealed in 2010 at Ulster the pressure peaking phenomenon (PPP) [5] is another unique of the e-Laboratory of Hydrogen Safety not available in other similar hazard and risk assessment software. It allows calculation of pressure dynamics in an enclosure like garage in case of unscheduled release of hydrogen. Both hydrogen blowdown release and constant mass flow rate release options are available. The tool is applicable for both ignited (fire from TPRD) and unignited (TPRD failure) releases.

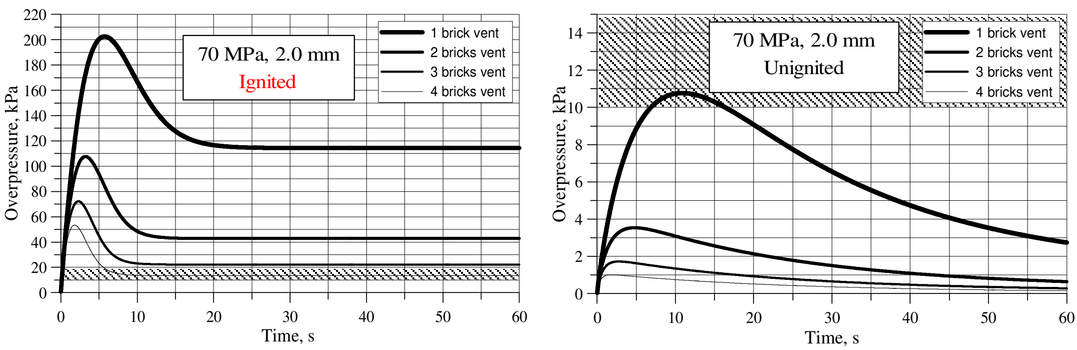

Fig. 4. Overpressure dynamics of hydrogen jet fire in the garage: TPRD diameter 2 mm and storage pressure 70 MPa (release rate 107 g/s) Ignited (left) vs unignited (right) [6].

The pressure peaking phenomenon is characteristic only for gases lighter than air when they are released into an enclosure with limited area of vents. The PPP is more pronounced for ignited release compared to unignited release from the same source [6], see Fig. 4. ISO standard requires the PPP to be taken into account when performing hydrogen safety engineering for indoor use of hydrogen and fuel cell systems.

The prevention and mitigation of the PPP can be achieved only through the decrease of mass flow rate from TPRD, i.e. its nozzle diameter. This is turn will require higher fire resistance rating of on-board storage tanks.

JET FIRE HAZARD DISTANCES

The “Jet fire” tool uses the dimensionless hydrogen flame length correlation [3] to calculate three hazard distances, i.e. “no harm” distance to T=70°C, which is 3.5 times of flame length; “pain limit” (115°C, 5 min), which is 3 times of flame length; and “fatality limit” (309°C, 20 s), which is 2 times of flame length. The universal flame length correlation includes laminar and turbulent flames, buoyancy- and momentum-controlled fires, expanded (subsonic and sonic) and under-expanded (sonic and supersonic) jet fires, thereby covering the entire spectrum of hydrogen reacting leaks [3]. Theoretical and experimental results indicate that the flame length has to be a function of not only the Froude number (*Fr*) but also the Reynolds (*Re*) number and the Mach (*M*) number and in this correlation, all are taken into account. One of its advantages is the absence of parameters at the notional nozzle exit, which are derived in the limited validity range assumption of sonic flow at the notional nozzle. The parameters needed to predict the flame length are those at the actual nozzle exit only: diameter, hydrogen density and flow velocity, the speed of sound at pressure and temperature at the real nozzle exit. The dimensionless correlation for hydrogen jet flame length in still air is L_F/D–$(\rho_N/\rho_S)\cdot(U_N/C_N)^3$ and shown in Fig. 5. Here L_F is the flame length, D is the nozzle diameter, ρ_N and ρ_S are release densities at the nozzle and surrounding air respectively, while U_N and C_N are velocity at the nozzle and speed of sound in the released gas in the nozzle.

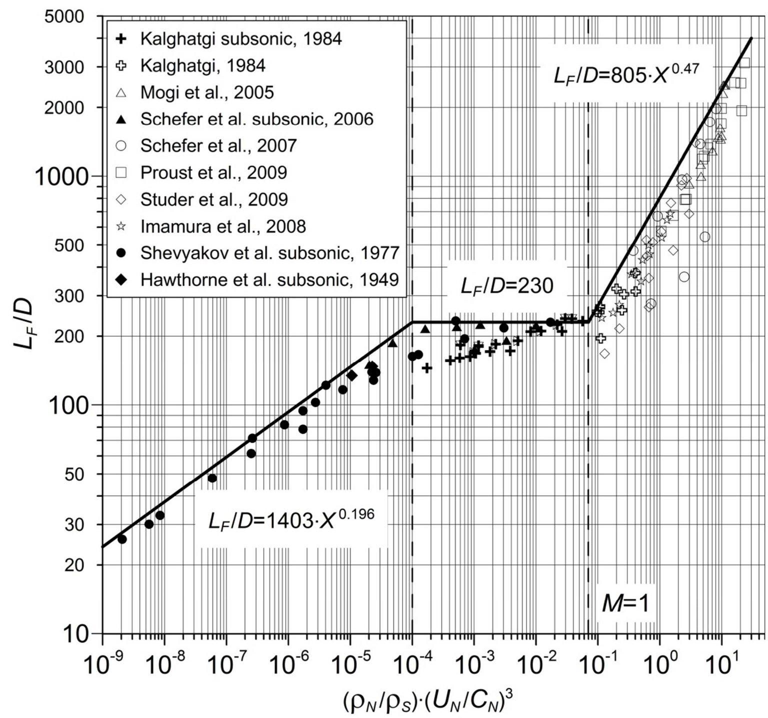

Fig. 5. Dimensionless flame length correlation [3].

The use of the correlation requires application of an under-expanded jet theory to calculate these parameters. There is lesser uncertainty in calculation of flow parameters in the actual nozzle exit compared to uncertainties at the notional nozzle. Indeed, there is a strong non-uniformity of velocity downstream of the Mach disk that deviates from the common for all under-expanded jet theories assumption of uniform velocity at the notional nozzle exit.

Mitigation of deflagrations

There are three deflagration mitigation tools in e-Laboratory of Hydrogen Safety: vent sizing of enclosure with uniform hydrogen-air mixture [7], vent sizing of enclosure with localised non-uniform mixture [8], calculation of upper limit of hydrogen inventory that can be allowed in a closed space like warehouse [8].

The vent sizing correlation for the uniform hydrogen-air mixture in vented enclosure [7] is based on recent advancements in understanding and modelling of combustion phenomena relevant to hydrogen–air vented deflagrations and unique large-scale tests carried out by different research groups. The combustion phenomena accounted for by the correlation include: turbulence generated by the flame front itself; leading point mechanism stemming from the preferential diffusion of hydrogen in air in stretched flames; growth of the fractal area of the turbulent flame surface; initial turbulence in the flammable mixture; as well as effects of enclosure aspect ratio and presence of obstacles. The tool allows to calculate the vent area to reduce the deflagration pressure to the desired limit and estimate the overpressure inside vented enclosure for the vent of given size.

The model for localised non-uniform mixture [8] describes deflagrations of hydrogen-air mixtures and defines safety requirements for vented deflagrations of localised mixtures in an enclosure. Examples of localised mixtures include ‘pockets’ of gas within an enclosure as well as stratified gas distributions which are especially relevant to hydrogen releases. It allows to estimate the maximum overpressure inside vented enclosure as well as calculating the vent size in order not to exceed the required safety limit.

Thermodynamic model to predict maximum mass of hydrogen, which may be allowed to be released in an enclosure of particular volume without causing destructive deflagration overpressure was developed [8] and realised as a tool in e-Laboratory. The model presumes that an enclosure is partially filled with air and hydrogen-air mixture. If this hydrogen-air mixture is burnt in a sealed enclosure, the model solution for resulting absolute pressure may be found. The tool allows to calculate the inventory mass for the given overpressure and enclosure volume for the given overpressure and inventory mass.

Blast wave and fireball after tank rupture in a fire

The “Blast wave” overpressure decay tool is available for stand-alone and under-vehicle storage tank scenarios. The model developed accounts for the real gas effects and combustion of the flammable gas released into the air (chemical energy) as a contribution into the blast wave strength [9]. The chemical energy of combustion is dynamically added to the mechanical energy and is accounted for in the energy-scaled non-dimensional distance. The model can be applied as a safety engineering tool for typical hydrogen storage applications, including on-board vehicle storage tanks and a stand-alone refuelling station storage tanks. The predictive model is required for calculation of hazard distances defined by the parameters of a blast wave, which is generated by a high-pressure gas storage tank rupture in a fire.

The tool for calculation of “Fireball” diameter after hydrogen tank rupture in a fire is based on the assumption of complete combustion of released hydrogen in air [9], [10]. It is based on limited amount of experimental data and thus requires further validation.

CONCLUSIONS

The scientific principles behind engineering tools of the e-Laboratory of Hydrogen Safety are overviewed. They predict a wide range of realistic phenomena related to hydrogen safety engineering not limited to assessment of overpressures caused by pressure peaking, deflagration and tank explosion, concentration of hydrogen in the jet and indoors, temperature along the jet fire, parameters of the jet and others. The developed engineering tools are being implemented for the stakeholders' free access in the e-Laboratory of the NET-Tools project. All principles behind the implemented online tools of e-Laboratory are based on peer-review publications and their ability to reproduce the results of future experiments is tested and widely validated in order to predict most of accidents related to hydrogen storage, production and distribution and help to develop safety solutions. The e-Laboratory of Hydrogen Safety has the largest number of tools for calculation of hydrogen hazards compared to other similar tools being developed in North America, including but not limited to unignited and ignited released in the open and confined spaces, mitigation of deflagrations, assessment of blast wave and fireball after high-pressure hydrogen tank storage in a fire, etc.

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