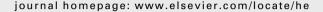
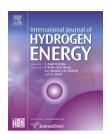


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An inter-comparison exercise on CFD model capabilities to predict a hydrogen explosion in a simulated vehicle refuelling environment

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ABSTRACT

The paper describes the comparison of simulations of a hydrogen explosion experiment in an environment simulating a vehicle refuelling station. The exercise was performed in 2007 within the European Commission-funded Network of Excellence "Hydrogen Safety as an Energy Carrier" (http://www.hysafe.org), which facilitates the safe introduction of hydrogen technologies and infrastructure. The experiment in a mock-up of a hydrogen refuelling station was conducted jointly by Shell Global Solutions (UK) and the Health and Safety Laboratory (UK) in order to study the potential hazards and consequences associated with a hydrogen-air mixture explosion. The "worst-case" scenario of a stoichiometric hydrogen-air mixture explosion was offered to the network partners for this simulation exercise. Simulations were conducted by a total of seven partners using different models and numerical codes with the intention of predicting/reproducing pressure dynamics in different locations and of evaluating the performance of different combustion codes and models in realistic large-scale conditions. The paper briefly details the models and numerical codes used, and presents the simulated pressure transients obtained by the partners in comparison with the experimental pressure records. The comparative model analysis was made based on achieved simulation results, where the simulated maximum overpressure and the characteristic rate of pressure rise were treated as major output parameters. A contribution to hydrogen safety was made in the form of a description of the models, their performance and an analysis of the results for their cross-fertilisation where possible.

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1. Introduction

There is a potential for introducing hydrogen as an energy carrier into the consumer market in the near future, particularly in transport applications. One aspect that needs to be addressed is the safety issues of hydrogen storage, transport and infrastructure. The European Network of Excellence "Hydrogen Safety as an Energy Carrier" (HySafe) is a project funded by the European Commission, which focuses on improvement and coordination of the knowledge and understanding of hydrogen safety and supporting the safe and efficient introduction and commercialisation of hydrogen [1]. Large laminar burning velocity of hydrogen (up to 3.50 m/s in NTP air) and wide flammability limits (4.1-74.8% vol.) [2] may make hydrogen explosions potentially more severe and potentially more frequent than explosions of hydrocarbons. Contemporary predictive tools for hydrogen safety engineering, such as computational fluid dynamics (CFD), are essential for design of safe hydrogen applications. Accordingly, the CFD combustion models and numerical codes should be assessed in application to simulations of the hydrogen explosions to demonstrate the credibility of the simulations, the level of performance and the required computer time for solution which one may expect.

The activities of HySafe include developing a concept of computational fluid dynamics (CFD) applications to the problems related to hydrogen safety, particularly establishment of a database of hydrogen release and explosion experiments for validation of CFD models and codes. The HySafe consortium partners identify, and subsequently upgrade on a regular basis, a set of standard benchmark exercise problems (SBEPs). These are available publicly as well as through the consortium, and describe experiments on hydrogen releases and distribution, jet fires, deflagrations and detonations. Institutions wishing to participate in this exercise perform SBEP simulations in order to predict or reproduce experimental data. Comparative assessment of the CFD code performance against available experimental data and results between partners gives an indication of the quality and suitability of the models, numerical codes and user practices for application to hydrogen safety problems. Examples of previous SBEP simulation results performed by HySafe partners and the analysis can be found in refs. [3,4]. A joint CFD simulation exercise is a useful tool for comparative codes assessment and similar examples may be found elsewhere, e.g., validation of CFD simulations against hydrogen combustion experiments in nuclear reactor environment has been described in ref. [5] and validation of simulations against large-scale industrial explosions has been performed in ref. [6].

A description of the 31.4% vol. hydrogen-air mixture deflagration experiment in a mock-up hydrogen refuelling station environment was offered to the HySafe consortium as a potential SBEP in 2006 by Shell Global Solutions (UK) and the Health and Safety Laboratory (UK). It was agreed that peak overpressures would be available to the modellers in December 2006, so the simulations submitted before that time would be treated (and denoted through the text of the paper further) as "blind". However, overpressure dynamics were not available until they were presented at the 2nd International

Conference on Hydrogen Safety in September 2007 [7]. This SBEP was attractive for HySafe partners as safety of refuelling stations, where hydrogen will be handled routinely by the general public, is of particular interest in the framework of the emerging hydrogen economy. The range of accidental scenarios, potential hazards and outstanding safety issues related to the hydrogen refuelling stations may be seen through recent publications on the subject, e.g. refs. [8,9].

2. Experiment details

Three series of hydrogen explosion experiments were conducted jointly by Shell Global Solutions (UK) and the Health and Safety Laboratory (UK) in different geometries: (a) a repeated pipe congested geometry; (b) a stack of dummy storage cylinders to represent high-pressure hydrogen storage; and (c) refuelling station congestion [10]. Experiments were conducted in a geometry representing refuelling station congestion with an ignited hydrogen jet released from a 400 bar pressure vessel, and with a premixed cloud explosion. One of the experiments with a premixed cloud explosion was offered to HySafe as a SBEP; the details of the experiment are reported in ref. [7].

The SBEP experiment was designed to represent the worstcase scenario of a stoichiometric hydrogen-air mixture explosion in an environment simulating a realistic retail station. The experimental facility is outlined in Fig. 1. The experimental rig consisted of a dummy vehicle, two dispenser units and a confining wall. The concrete confining wall was 4.2 m high, 0.6 m wide and 5.4 m long. The dispenser units were made of steel, had dimensions $L \times W = 0.9 \times 0.6 \, \text{m}$ in plane and 2.1 m high and were fixed to the concrete pad. The vehicle was also made of steel plates fixed to the steel frame. The passenger section of the vehicle was 1.7 m wide, 3.8 m long and 1.3 m high and was welded to prevent mixture penetration into it. The engine bay of the vehicle was 1.7 m wide, 0.8 high, 0.7 m long and was open from the bottom to allow it to be filled with a hydrogen-air mixture. The whole vehicle was standing on 0.3 m high supports representing wheels. The facility was surrounded by a 5.4 m wide, 6.0 m long and 2.5 m high metal frame, which was adjusted to the wall and was covered, together with the outside of the wall, by a 23 µm plastic film to retain the hydrogen-air mixture. The total volume of the hydrogen-air mixture contained under the plastic film with sealed dispensers and the passenger section was 70.16 m³, which corresponded to a 13.4% blockage ratio.

In the experiment involved the equivalence ratio of hydrogen–air mixture was 1.092 (31.4% vol. $\rm H_2$), the gas mixture temperature at the ignition moment was 28.9 °C, and relative humidity 42.1%. The mixture was ignited by a spark of about 50 mJ energy. In the experiment offered for SBEP the ignition source was located between the dispensers 1.3 m from the confining wall and 1.25 m above the ground as shown in Fig. 1.

The facility was equipped with transducers (series ETL-345F-375M 4 MPa, piezoresistive) and hydrophones (Brüel & Kjær 8103). The location of the transducers, whose pressure records were used in the SBEP exercise described later for comparison with simulated pressure dynamics, is shown in

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