Transition of Spontaneously Ignited Hydrogen Release into a Jet Fire

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Introduction

The issues of climate change and independence of energy supply stimulate search for alternative energy sources and energy carriers. Hydrogen is an ecologically clean alternative fuel, which can act as a carrier or storage for renewable sources of energy. Safety is the main barrier for the emerging hydrogen economy. Specific hazards associated with hydrogen as an energy carrier has to be first understood and then addressed by engineering design to provide safety of hydrogen technologies at least at the same level as for traditional fossil fuels.

While mass-related energy density of hydrogen is higher compared to other fuels, it is impractical to store hydrogen under normal temperature and pressure. Thus, practical applications, such as hydrogen powered vehicles, require hydrogen to be compressed or liquefied. The pressure of hydrogen in onboard storage reaches 700 bar already and the refuelling stations for such storage operate at even higher pressures. A leak from such high pressure storage can lead to formation of highly underexpanded jet that in turn implies potential fire and explosion hazards and associated risks.

It is well-known that sudden hydrogen release from high-pressure vessel into air can be spontaneously ignited without any apparent ignition sources present, such as spark, hot surface, fire, etc. Spontaneous ignition of high-pressure hydrogen release is one of the main unresolved problems of hydrogen safety, for which little fundamental explanation exists. Many attempts have been made to explain this phenomenon over the last decades starting from pioneering study of Wolanski and Wojcicki in 1972 of the so-called “diffusion ignition mechanism” [1]. Up-to-date experimental data give critical conditions of the phenomenon, although they are quite scattered and depend on experimental setup. Unfortunately, they can not give a detailed insight into the dynamics of this physical process, for example exact location of initial ignition spots and progression of chemical reaction within tubing downstream the rupture disk or valve.

The main objective of this study is an insight into physical phenomena underlying spontaneous ignition of hydrogen at sudden release from high pressure storage and its transition into the sustained jet fire. This work describes modelling and large eddy simulation (LES) of spontaneous ignition dynamics in a tube with a rupture disk separating high pressure hydrogen storage and the atmosphere. It is demonstrated that a chemical reaction commences in a boundary layer within the tube, and propagates throughout the tube cross-section after that. Simulated by the LES model dynamics of flame formation outside the tube has reproduced experimental observation of combustion by high-speed photography, including vortex induced “flame separation”.

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Model

The LES technique is the most promising computational fluid dynamics (CFD) approach to solve scientific and engineering problems, including those related to hydrogen safety. Different LES models were developed previously and successfully applied to model deflagrations [2], detonations [3], non-reacting underexpanded jets [4], and jet fires [5]. The set of main governing equations can be found elsewhere [2]. In present study the RNG model was employed for subgrid-scale modelling of turbulence. The reaction rate that appears in species transport equation was modelled using eddy-dissipation-concept model by Magnussen [6]. It incorporates detailed Arrhenius chemical kinetics in turbulent flames. In this study the detailed 21-step chemical reaction mechanism of hydrogen combustion in air employing 37 elementary reactions by Gutheil et al. is applied [7].

Spontaneous ignition following burst-disk rupture

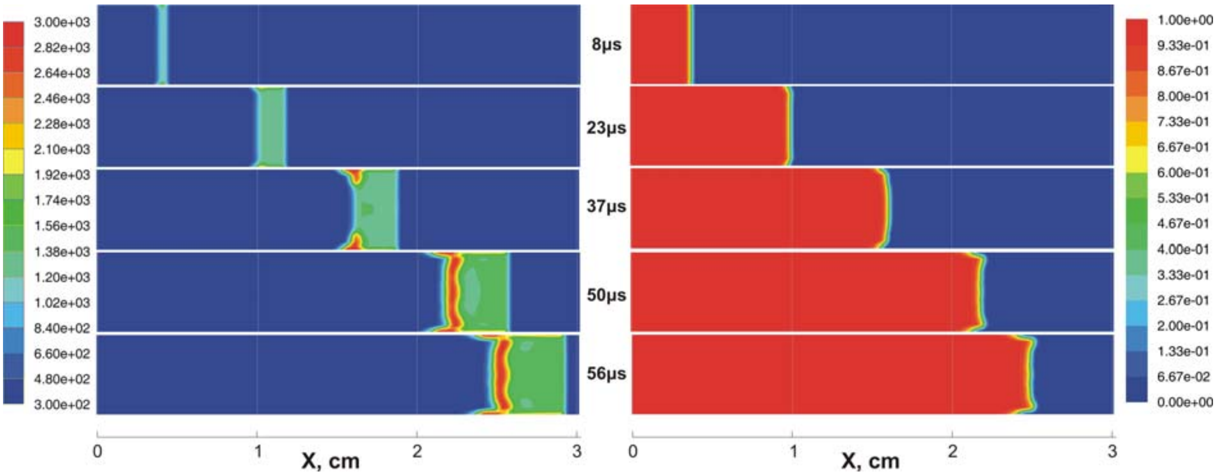

Figure 1. Dynamics of spontaneous ignition inside of the 5 mm ID tube temperature (left) and hydrogen mole fraction (right). Initial hydrogen pressure 97.6 MPa

The experimental data used for the LES model validation are those published by Golub et al. [8]. The experimental setup chosen for validation includes a high-pressure chamber filled with hydrogen to 97.6 MPa, and a low-pressure chamber with air at atmospheric conditions connected by a tube of 5 mm internal diameter and length up to 185mm. The chambers were separated by a copper burst disk. When the pressure in the high-pressure chamber exceeds the critical value, the burst disk ruptures and shock wave propagates through the low-pressure chamber (tube). In numerical simulations the reaction front is established throughout the pipe cross-section at distance 20 mm from the burst disk at time 45 μs after the instantaneous rupture. In the experiment the light and pressure sensors were located 33 mm from the burst disk. However, the time of the shock arrival was not reported. In LES the leading shock reached the light sensor location of 33 mm at 58 μs, and the reaction front followed the shock with a delay 7-10 μs. In the experiment the sensor started to register light 18-24 μs after the shock arrival.

Transition of spontaneous ignition into a jet fire

Sequence of photographs was obtained by Mogi et al [9] using high-speed digital colour video camera. Initial pressure of hydrogen in chosen for numerical simulations experiment was 14.5 MPa and the tube length was 185mm. This sequence of snapshots shows combustion of hydrogen-air mixture spontaneously ignited inside of the tube and then emerging outside and stabilizing in the vicinity of the tube exit. The authors [9] observed that, once the emerged from the tube flame is stabilized near the nozzle, it acts as a pilot flame and ignites/sustains the jet fire later on. Therefore, the numerical observation of flame "stabilization" near the tube exit may be taken as an indication of transition from the spontaneous ignition to the sustained jet fire.

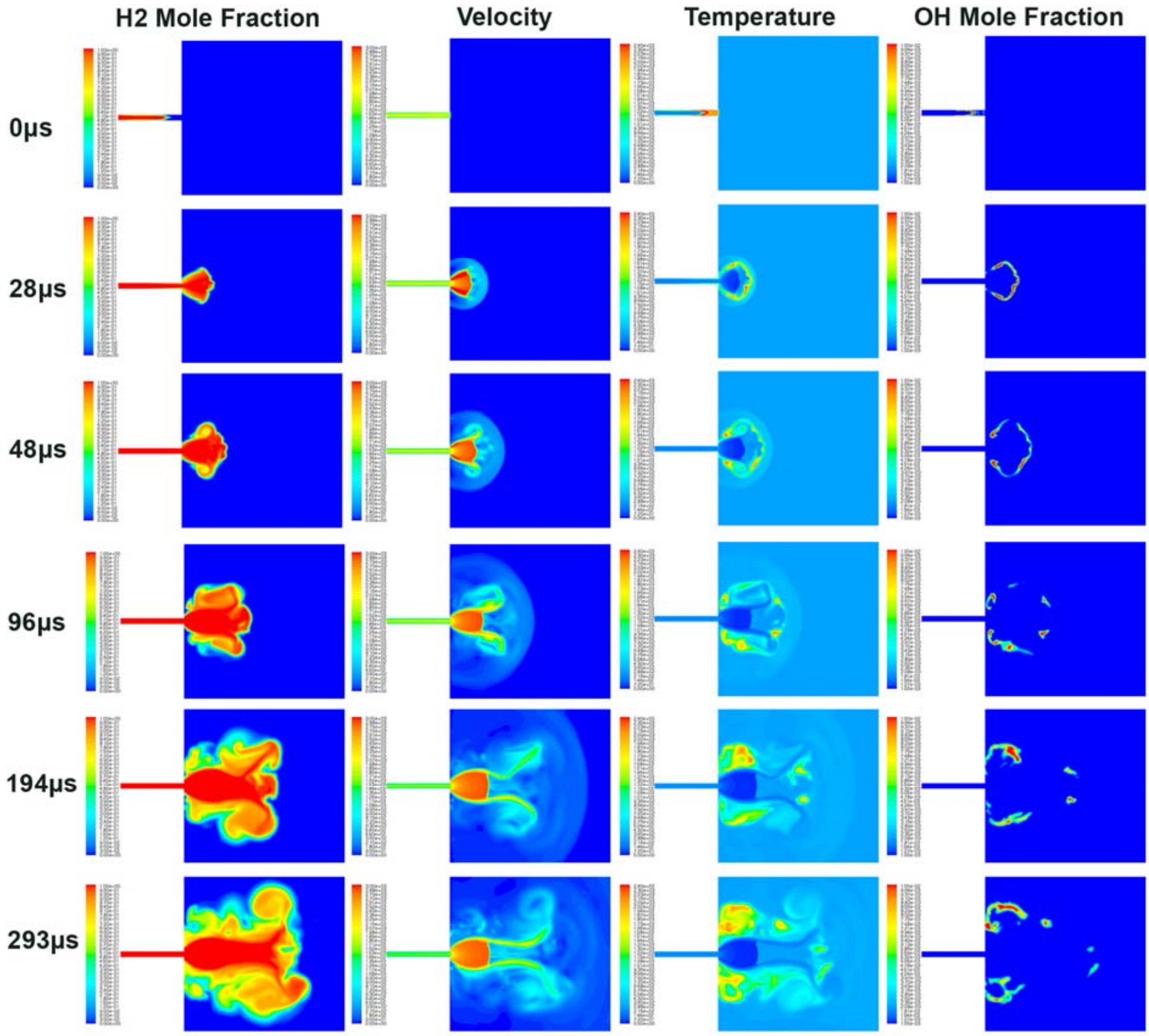

Figure 2. Dynamics of the velocity, temperature and mole fractions of hydrogen and hydroxyl during release from tube outside (2D slice along the tube axis). Initial hydrogen pressure 14.5 MPa, Tube length L = 185 mm, ID = 5 mm

Conclusions

The LES model for numerical simulation of spontaneous ignition of high-pressure hydrogen release into downstream attachment filled with air at atmospheric conditions and dynamics of combustion outside the attachment is presented. The mechanism of spontaneous ignition in tubes downstream of a pressure relief device, e.g. the rupture disk, is investigated. Numerical experiments have demonstrated that ignition is initiated in a wall boundary layer. Results of simulations are in agreement with experimental data on the distance for spontaneous ignition from the rupture disk.

The mechanism of transition from spontaneous ignition inside of the tube into sustained jet fire is studied within computational limitations. It is assumed, following the experimental observations, that the transition to the sustained jet flame is largely dependent on the initial jet formation stage, where developing annular vortex pushes combusting mixture upstream into the recirculation zone. Once the flame is stabilised near the tube exit, it acts as a pilot flame and ignites jet fire later on. The LES model validated against experimental data can be used for engineering design of innovative pressure relief devices.

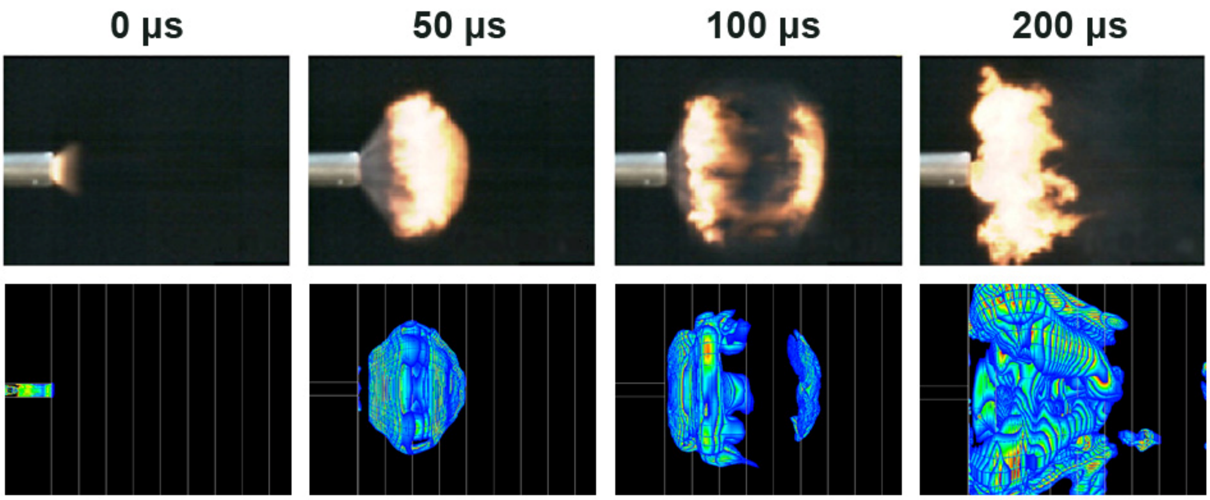

Figure 3. Comparison of high-speed video camera experimental photographs obtained by Mogi et al. [9] with numerical LES snapshots.

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