Research paper

Influence of geometrical configuration on spontaneous hydrogen ignition process

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Abstract

Hydrogen is considered as a future fuel which may replace traditional ones. There are several arguments for utilization of the hydrogen : high heat of combustion, zero CO_2 emission, etc. But there are also significant disadvantages : low density, high cost of production and safety problems.

Nowadays, hydrogen, used in vehicles, can be stored at pressure up to 70 MPa, but high pressure discharge of the hydrogen into atmosphere can cause spontaneous ignition, so a failure of any element of high pressure hydrogen installation generates hazard of potential fire and explosion.

The experimental research conducted in the Combustion Laboratory, Institute of Heat Engineering, Warsaw University of Technology gave new data concerning influence of the geometry of the extension tube on the hydrogen ignition process. In the experimental investigation it was confirmed, that the process of hydrogen ignition is stochastic in nature, since it depends upon many parameters. One, which is very difficult to control, is the process concerned with bursting of the diaphragm that closes high pressure hydrogen container. In the paper, a comparison is presented of the experimental results obtained in the Combustion Laboratory of Warsaw University of Technology with numerical simulations conducted at the Dept. of Aerospace, University of Michigan.

Keywords : hydrogen, safety, ignition.

1. Introduction

The first investigations concerned with the problem of ignition of hydrogen during an outflow from high pressure installation were carried out nearly 40 years ago by Wolanski and Wojcicki[1)−3)]. The research was mainly aimed at determining the source of the ignition in a tragic accident in Chorzow Chemical Plant „Azoty", where explosion of synthesis gas (hydrogen−nitrogen mixture, 3 H_2—N_2, 300 °C, 30 MPa) killed four people. More recently, there were several other reports on high pressure hydrogen leaks resulted with ignition without an external ignition source[4)−7)].

Hydrogen is regarded as a perspective fuel for various kinds of vehicles : fuel cell cars, trucks, buses etc. Storing and transportation constitute crucial safety problems concerned with utilization of hydrogen as a vehicle fuel. Because of its low density in gas phase, hydrogen needs to be stored under very high pressure or in a liquid state. The latter storage system is much more complex and expensive, so the former one probably will be more commonly utilized in vehicles. It is anticipated that vehicle hydrogen tank pressure will be equal to 35, 70 or even 100 MPa.

High pressure of stored hydrogen causes a potential risk of sudden rapture of a tank or a high pressure installation, which can lead to ignition and a potential explosion. Mixing of hydrogen with the air heated up by a shock wave generated by expanding hydrogen can result in ignition of a formed combustible mixture. Numerous papers on numerical and experimental investigations concerned with hydrogen safety and the high pressure hydrogen outflow ignition were recently published[8)−14)].

In the experimental research, the process of hydrogen discharge is usually initiated by burst of a diaphragm closing high pressure hydrogen container. The process of the diaphragm burst generates more or less intensive turbulization of the hydrogen outflow, what has a significant influence on the mixing of hydrogen and the air compressed and heated up by the shock wave. In every conducted test the diaphragm bursts in slightly different way, what has a strong influence on the repeatability of the test results.

The aim of this research was the investigation into influence of geometrical configuration and the way the diaphragm bursts upon the process of hydrogen ignition during the outflow from high pressure installation.

2. Experimental research

The experimental tests were conducted on a facility constructed in the Combustion Laboratory of the Institute of Heat Engineering, Warsaw University of Technology.

The facility[13] consists of two main elements: a high pressure hydrogen container and a visualization chamber. Both, the hydrogen container and the visualization chamber are equipped with pressure transducers. The visualization chamber is additionally equipped with a photodiode reacting to the flame.

The high pressure hydrogen container is closed by a plastic diaphragm which bursts when the pressure inside the container reaches the determined value. An extension tube can be attached to the container. Extension tubes of various geometries were tested in experimental and numerical investigations[4)–6)]. The extension tube, tested in the presented research, consisted of two parts[13]: the first one of 10 mm of diameter and 10 mm of length placed just behind the diaphragm, and the other one, with various diameters and various lengths, connected to the first one. Between the first part and the diaphragm there is a conical channel which helps to control the process of the diaphragm burst. The flow and the ignition of hydrogen after the discharge were registered with use of high speed digital camera Photron Fastcam SA1.1. Pictures were taken directly or with use of Schlieren system[13].

3. Numerical simulations

Numerical calculations were conducted with use of Fluent 6.3.26 software. The 2D, axis symmetric computational domain was generated with use of Gambit 2.3.16 and is shown in Fig. 1. The extension tube consisted of two parts: the first one of 10 mm of diameter and 10 mm of length placed just behind the diaphragm, and the other one, with 25 mm of diameter and 45 mm of length, connected to the first one. The diaphragm separates high pressure hydrogen and ambient pressure air. The size of the mesh cells of the grid in the proximity of the diaphragm location was in order of 50 μm.

In the experimental tests, the diaphragm expands and bursts inside the extension tube in various ways. The different ways of the diaphragm burst were modeled by a change of the initial geometrical conditions of the numerical computations. The calculations were conducted for various positions of the diaphragm separating high pressure hydrogen from ambient pressure air. The main aim of the calculations was to investigate influence of the initial conditions on the process of hydrogen ignition. Figure 2 presents two of tested positions of the diaphragm. In the initial condition 1 the diaphragm is located on the edge of the conical part of the tube, and in the initial condition 2 the diaphragm is located 1 mm from the edge of the conical part

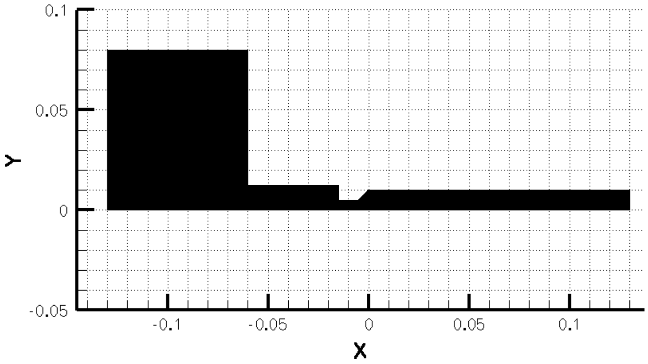

Fig. 1 Geometry of the numerical domain.

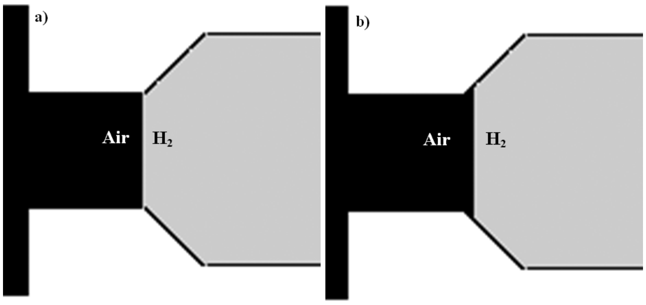

Fig. 2 Numerical domain in proximity of the diaphragm location.
a) Initial condition 1
b) Initial condition 2

It was found that the use of simplified, one reaction mechanism gives unrealistic results and underestimates critical hydrogen pressure required for the ignition. It was a preliminary stage of the numerical investigation. In the presented computations, the following 5 reactions model of the hydrogen combustion was utilized:

$$\begin{gathered} H_2 + O_2 = HO_2 + H \\ H + O_2 = OH + O \\ O + H_2 = OH + H \\ OH + H_2 = H + H_2O \\ H + O_2 + M = HO_2 + M \end{gathered}$$

In the conducted computations standard k−ε turbulence model was used.

Pictures in Fig. 3 and Fig. 4 present distributions of temperature and OH concentration in the end of the extension tube obtained from the simulations. The direct pictures recorded during the experimental test, conducted with described above geometry of the extension tube, are compared with the results of the numerical computations. Initial hydrogen pressure was equal to 7.6 MPa.

As it can be seen on the presented figures, the general shape of the hydrogen flame is qualitetively reconstructed by the numerical model. It is also clear that the initial conditions have significant influence not only on the

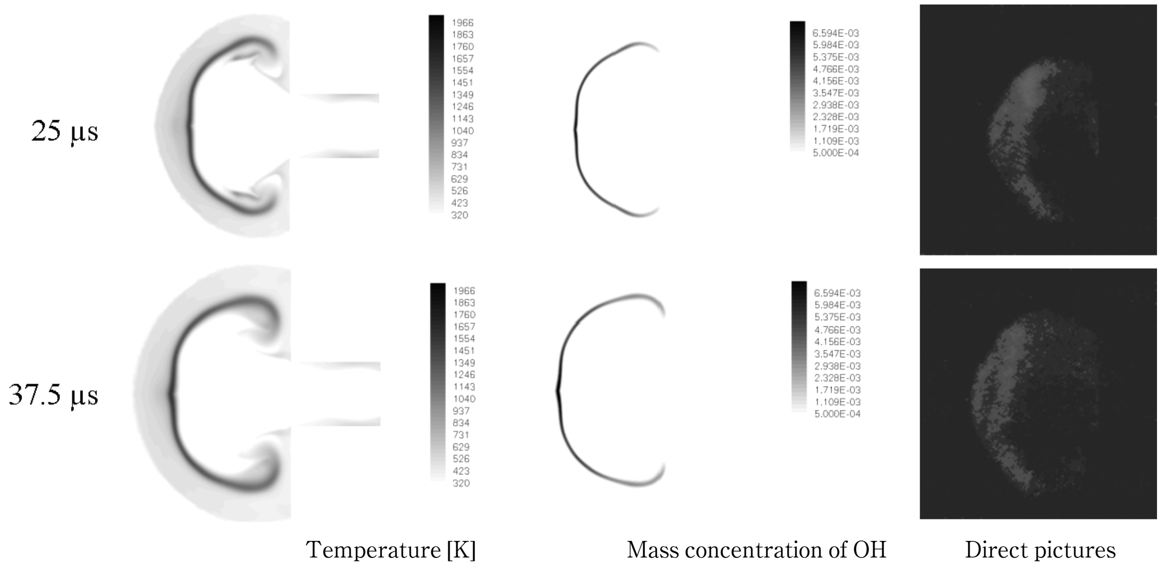

Fig. 3 Comparison of experimental results with numerical computations, the extension tube length equal to 45 mm, the extension tube diameter equal to 25 mm, hydrogen initial pressure equal to 7.6 MPa. Numerical computations—initial conditions 1, temperature and OH concentration distributions, experimental results —direct pictures, 80,000 f/s. Time step between pictures equal to 12.5 μs.

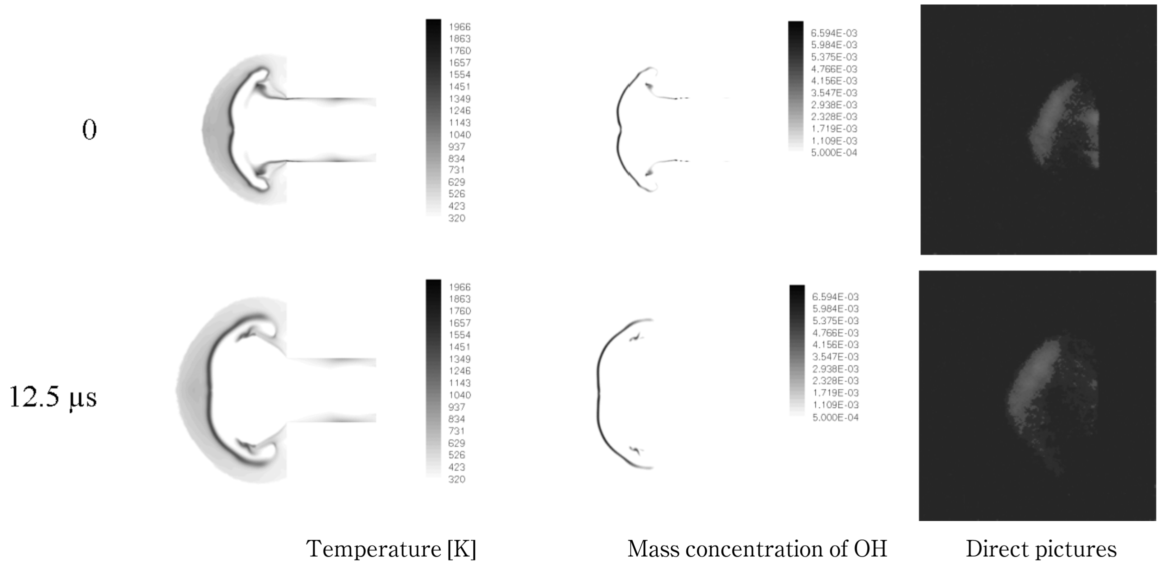

Fig. 4 Comparison of experimental results with numerical computations, the extension tube length equal to 45 mm, the extension tube diameter equal to 25 mm, hydrogen initial pressure equal to 7.6 MPa. Numerical computations—initial conditions 2, temperature and OH concentration distributions, experimental results —direct pictures, 80,000 f/s. Time step between pictures equal to 12.5 μs.

occurance of the ignition but also on the further flame propagation.

Comparisons of the pictures presented in Fig. 3 and Fig. 4 lead to conclusion that initial conditions 2 give the shape of the flame front more similar to the experimental result.

The initial conditions 2 generate more turbulized flow with the ignition taking place on the edge of the conical part of the extension tube.

Figure 5 presents map of results of further research obtained for various hydrogen initial pressure values and different initial conditions. Pictures below graph present three tested geometries of hydrogen−air boundary : initial condition 1 and initial condition 2, presented above and a membrane initial condition. In the membrane initial condition it is assumed that in the experiment the membrane initially expands and then it busts. The numerical results are also compared with the experimental tests. As it can be seen on the presented graph results obtained with use of initial condition 2 gives the lowest critical value of hydrogen pressure required for ignition and this critical value is very close to that obtained in the experiments.

4. Conclusions

The results of the experimental tests and numerical simulations show that geometry of the extension tube and the process of the diaphragm opening have a significant influence on the presence of the hydrogen ignition and the flame propagation.

In general, the ignition process shows a stochastic behavior, as it depends very much on random processes associated with opening of the diaphragm (membrane). The numerical model used in the research enables to

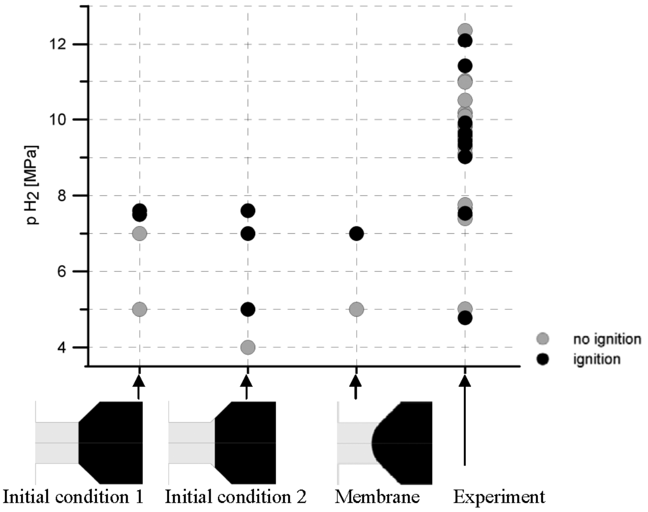

Fig. 5 Results of the numerical results as a function of the initial conditions. Comparison of the numerical results with experiments.

simulate the hydrogen ignition and flame propagation inside the extension tube and to investigate influence of the diaphragm initial location on the process. In order to investigate the potential consequences of the failure of the elements of real high pressure hydrogen installations and to explain a complicated nature of this phenomenon more research, both experimental and numerical is necessary.

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