

Auto-ignition of high pressure hydrogen release

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1 Introduction

Hydrogen is a renewable energy which could meet most of our future energy needs and reduce our reliance on oil. Nevertheless, in order to store or transport H₂ carefully, its safety issue has to be solved to utilize it within regulations. The current research concerns hydrogen safety, especially its auto-ignition problem. Wolanski and Wojcicki [1] were the first scientists who studied this phenomenon and demonstrated that the auto-ignition of hydrogen occurred due to the diffusion of mass and heat. When high pressure hydrogen is jetting into the atmosphere, a shock wave is produced in front of and at some distance away from the hydrogen jet front and heats the air between the shock front and the hydrogen jet front. Recently the high pressure hydrogen release through a tube was studied by several groups. In the case of tube the heat flux behind the shock wave heats up the combustible mixture at the hydrogen jet front and its side boundaries with the air to auto-ignite the mixture. The recent numerical simulations made by Liu et al. [2,3] show that the high pressure hydrogen spouting from a hole has a difficulty with its auto-ignition due to a strong expansion. The experimental study by Dryer et al. [4] suggests that the downstream geometry behind the jet seems to have an important influence whether the ignition is obtained or not. According to these remarks it was decided to study the hydrogen auto-ignition spouting from a tube.

Experimental and numerical studies are performed to clarify the mechanism of hydrogen auto-ignition spouting from a tube. Several different types of tube configurations are applied experimentally to see the limit of auto-ignition of hydrogen in these conditions. Numerical investigation is also performed to understand the mechanism of hydrogen auto-ignition. Especially the important parameters of hydrogen auto-ignition are investigated: the hydrogen pressure, tube diameter, tube length, and tube inner surface configuration.

2 Experimental method

2.1 Apparatus

The aim of the experiment is to observe the auto-ignition of a high pressure hydrogen jet and to make clear its mechanism. As shown in Fig. 1, hydrogen is compressed using a small shock tube. At the end of the low pressure section, a diaphragm provides the desired hydrogen jet pressure. Nitrogen gas is injected at the pressure of 5 or 8 MPa into the high pressure section of the shock tube upstream the piston to push it toward hydrogen gas. This piston compresses the hydrogen gas until a certain rupture pressure (P_r) ($2.7 < P_r < 6.9$) is reached. As the diaphragm is ruptured, the hydrogen gas is jetting into a dump tank at atmospheric pressure. The characteristics of this supersonic jet and the inflammation provide in some case in this jet are studied using pressure measurements, self-emission photos (coming from the ICCD camera with five nanosecond shutter

speed (La Vision)), and high speed movies (coming from a Shimazu high speed camera with one million frames per second).

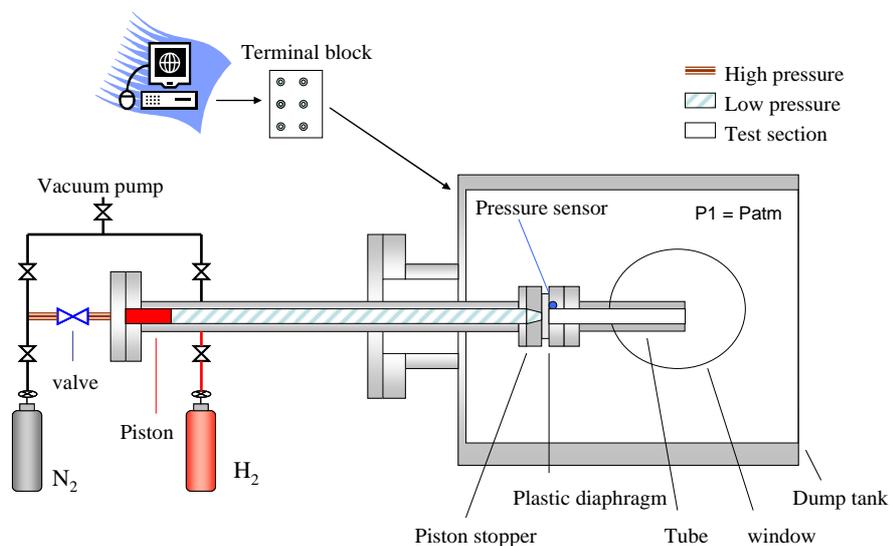


Figure 1 Experimental set-up

2.2 Experimental conditions

The experiments consist of observing hydrogen auto-ignition by varying several parameters. First, the hydrogen pressure by using different kinds of diaphragm thickness. Second, the geometry downstream the diaphragm that consists of different kinds of tube: straight and screwed tubes. Straight tube diameters are 4.8 and 10 mm and for the screwed tube, it is 10.3 mm. The screwed tube consist in a straight tube where inside screw have been made. For each case, several tube lengths are tested at different pressures of H₂: 48, 71, and 113 mm for 4.8 mm diameter tube; 50, 100, 118, 180 mm for 10.0 mm diameter tube and 50, 100, 118, 180 mm for 10.3 mm diameter tube.

3 Numerical method

The governing equations are the compressible two-dimensional axisymmetric Navier-Stokes equations, the conservation equations of total energy and chemical species, and the equation of state. The equation of total mass conservation is solved additionally. A chemical reaction model by Petersen and Hanson [5] with 9 species (H₂, O₂, O, H, OH, HO₂, H₂O₂, H₂O, and N₂) and 18 reactions is used to solve the present problem. This reduced kinetics mechanism has good performance of ignition delay time and heat release within a wide pressure range from 1 to 600 atm. The air is assumed to be composed of 22% O₂ and 78% N₂ in volume. The diffusion flux is evaluated using Fick's law with binary diffusion coefficients. The transport coefficients of each chemical species: viscosity, heat conductivity, and binary diffusion coefficient, are evaluated using the Lennard-Jones intermolecular potential model [6], and those of the gas mixture are calculated by Wilke's empirical rule [7]. The enthalpy of each chemical species is derived from NIST data base [8]. The buoyancy, bulk viscosity, Soret and Dufour effects are neglected.

The governing equations are discretized in a finite difference formulation. The convective terms are evaluated using the second-order Explicit Harten-Yee Non-MUSCL modified-flux type TVD scheme, considering the properties of the hyperbolic equations. The viscous terms are evaluated with the standard second-order central difference formulae. The time integration method is the second-order Strang-type fractional step method. The chemical reactions are treated by a point implicit method to avoid the stiffness.

The jet exit is on the same plane as the outside surface of the wall. These conditions are kept in the simulation. The computational domain is a rectangular zone with a length of 80-90 mm in x-direction and a width of 80-120 mm in y-direction. The x-direction is the jet axial direction. The left boundary is a solid wall with a hole located at its center. Non-slip conditions are imposed on the wall and the free stream conditions are applied to the other three boundaries. The flow is adiabatic. At the initial state, the computational region is filled with still air at 1 atmosphere and 300 K. No artificial disturbance is imposed. The grid system is rectangular and a uniform grid size of $dx = dy = 20 \mu\text{m}$ is accepted. The total grid number is 27 million.

4 Results and discussion

4.1 Auto-ignition characteristics for two kinds of tube configuration

The following Figs. 2 and 3 show the results obtained (ignition or not ignition) for two kinds of tube.

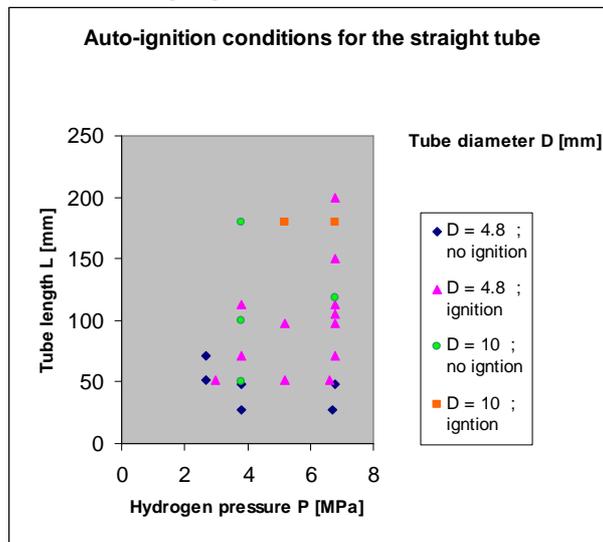


Figure 2 Auto-ignition conditions for straight tube

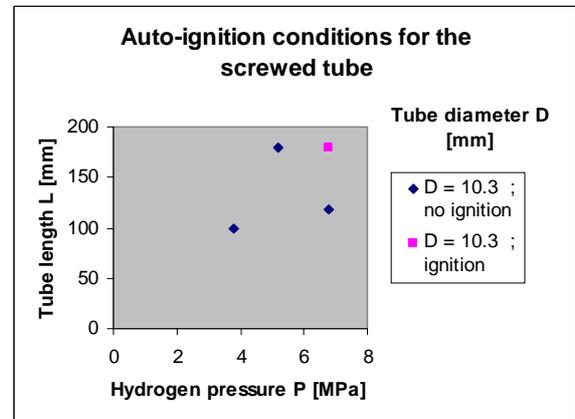


Figure 3 Auto-ignition conditions for screwed tube

From these results in Figs. 2 and 3 some limits are recognized for hydrogen pressure, tube diameter, and tube length. The higher hydrogen pressure makes its auto-ignition easier. The lower limit for hydrogen auto-ignition is reached just at 3 MPa with a straight tube length of at least 51 mm and a tube diameter of 4.8 mm. Experiments with the screwed tube are too few to draw some conclusions. However this screwed tube gives no ignition for the same conditions as the straight tube, a diameter of 10.0 mm, a hydrogen pressure of 5.2 MPa and a tube length of 118 mm. This implies that with the screwed tube it is harder to ignite high pressure hydrogen, because the jet temperature is cooled down by the rings.

The following Figs. 4 and 5 show a comparison between the experiment and numerical simulation of high pressure hydrogen jet spouting from the tube of 10.0 mm in diameter at the condition of 2.3 MPa hydrogen pressure for the experiment and 3.8 MPa hydrogen pressure for the numerical simulation.

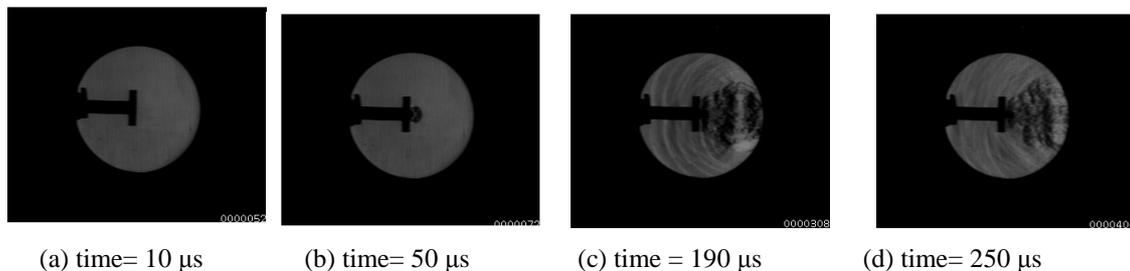


Fig. 4 Schlieren photos of high pressure hydrogen jet spouting from the straight tube of 10.0 mm in diameter and 118 mm in length at the hydrogen pressure of 2.3 MPa.

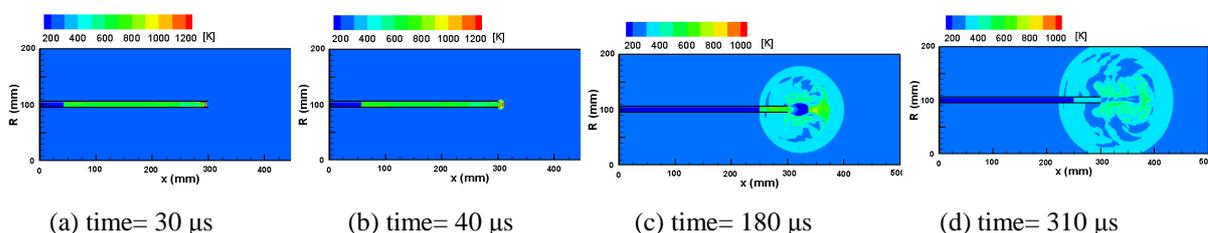


Fig. 5 Numerical simulation of temperature profiles of high pressure hydrogen jet spouting from the tube of 10.0 mm in diameter and 50.0 mm in length at the hydrogen pressure of 3.8 MPa.

5 Summary

High pressure hydrogen jet spouting out of different tubes are studied experimentally and numerically to clarify its auto-ignition mechanism and conditions. The hydrogen pressure, tube diameter, and tube length are important factors for hydrogen jet auto-ignition. As far as the straight tube is concerned, hydrogen jet does not ignite under 3.0 MPa in a tube of less than 51 mm in length, and of less than 4.8 mm in diameter. The screwed tube provides some difficulty for hydrogen auto-ignition, but the number of experiments is not enough large to draw any conclusion. The numerical calculations seem to give a good simulation, but some more one have to be done, with conditions matching with experiments.

References

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