Prevention of hydrogen self-ignition at technical opening via replacement of one orifice by several smaller ones

Tatyana V. Bazhenova, Victor V. Golub, Igor N. Laskin, Nikolay V. Semin,

Department of Physical Gas Dynamics,

JIHT of Russian Academy of Sciences, 125412, Moscow, Russia

1 Introduction

Motivation for safety investigation of hydrogen is connected with the global trend to find alternative energy sources as a replacement for conventional fuels. In several fields, for instance chemical industry, hydrogen has been safely produced, distributed, and used for many decades. However, the developed safety procedures and technologies provide only limited guidance for future stationary and mobile hydrogen applications. Namely, in the case of hydrogen powered vehicles, hydrogen will be utilized within a decentralized infrastructure in relatively small amounts (several kg per user) by a large population without special training in the safety of combustible gases [1]. The public will only accept future hydrogen technologies, if a safety level comparable to that of current technologies can be obtained.

In the review by Astbury and Hawksworth [2] a rigorous research was done on accidents involving spontaneous ignition of hydrogen at high pressure. Over the last century, 81 major accidents were reported. It turned out that in 86% of cases there was no clearly identifiable ignition source. Several mechanisms have been postulated as responsible ones for this phenomenon, for example, reverse Joule-Tompson effect, electrostatic ignition, sudden adiabatic compression. However, none of these causes could stand up detailed scientific analysis except one. In 1973, Wolański and Wójcicki observed that hydrogen heated below the auto-ignition threshold could ignite if it was released into a open space with oxigen or air. They demonstrated that ignition occurred due to high jump in temperature on the contact surface, where heated by a primary shock wave oxigen mixed and reacted with hydrogen due to diffusion. Thus, for the first time, diffusion self-ignition mechanism was proposed [3]. Recently, this scenario attracted lots of interests as a possible cause for industrial hazards [4-8].

Unlike in the experiment conducted by Wolański and Wójcicki, Baev [4] poured hydrogen into a partly closed tube preliminary heating it. Howeverm, the tube had several obstacles, and hydrogen self-ignition was observed only after a shock wave reflected from the obstacles. In the investigation by Mogi [5] ruptured disk was used in the rapid discharge of high-pressure hydrogen into a tube 5-10 mm in diameter with an open end. The faiture pressure was changed from 40 to 400 bar. Ignition of the hydrogen jet was observed in the extension tube. The paper of Dryer [6] reports the similar mechanism of hydrogen and natural gas self-ignition at the burst disk failure and combustible gas release into the tube filled with air. Furthermore. the transverse shocks formed the burst disk failure leaded to heating of the gas on the contact surface. Golub [7] the self-ignition of high-pressure hydrogen in the tubes of

Correspondence to: golub@ihed.ras.ru

round and rectangular cross sections is investigated experimentally and numerically. Mechanisms leading to hydrogen self-ignition in the tube have been determined.

Previously, most of works devoted to hydrogen safety investigated discharge into tubes or confined space. The aim of this investigation is a numerical study of boundary phenomena influence on the hydrogen self-ignition at the discharge into the semi-confined space.

2 New concept for pressure release valve nozzle design

In paper [8], numerical modeling of hydrogen jet has been conducted where hydrogen jetted into atmosphere through a symmetrical orifice in 2D case. Dependence of flame occurrence on orifice diameter has been obtained. It turned out that for diameter smaller than 2.6 mm the ignition did not started or died out fast, hydrogen pressure being up to 400 atm.

Based on the result of this work, an idea to replace a big release valve nozzle by several smaller nozzles of the same total area emerged. Consequently, in case of accidental high pressure hydrogen release there is hope the ignition won't occur if boundary condition has been properly set. Namely, the diameter of the small orifices and the distance between them are matched in a way that every small orifice behaves like an isolated one, so that the ignition is inhibited due to rarefaction waves.

3 Numerical modeling of hydrogen jetted into atmosphere

Investigation of hydrogen jetting into the semi-confined space from a high pressure vessel was numerically simulated in the axisymmetrical two-dimensional (2D) case and in the three-dimensional (3D) case. Different geometry of technical openings has been studied, but overall area of the openings was the same in all cases. In particular, we have compared hydrogen release from one orifice of 4 mm in diameter and a system of 4 identical orifices with the diameter of 2 mm each. The total area was 16π mm^2 in both cases. The system of 4 identical orifices represented 4 circular holes, placed in the verticies of a square. The length of the square side – L – was a varying parameter in the calculations.

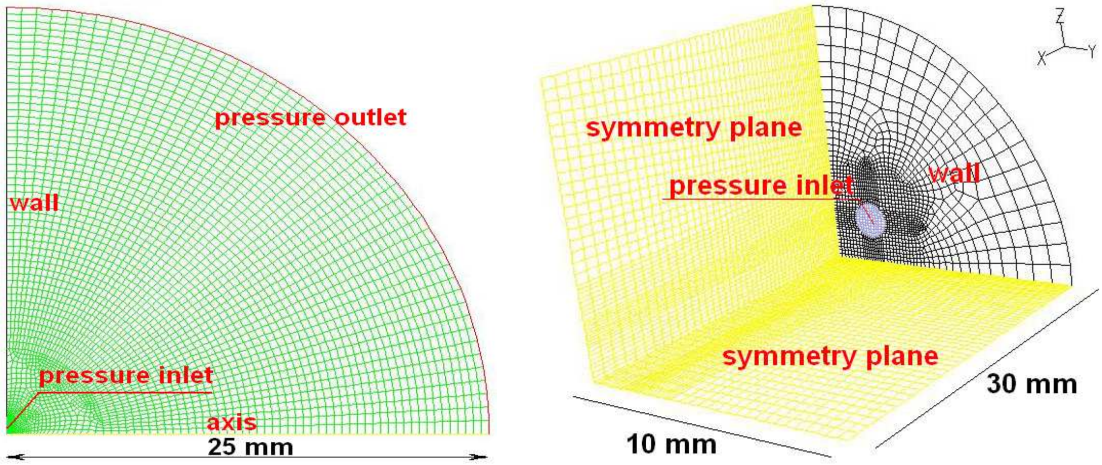

Figure 1. Computational grid in 2D (left) and 3D (right) cases.

The numerical modeling of the self-ignition of a hydrogen jet was performed based on the full system of Navier-Stokes equations for the multicomponent mixture of gases [9]. Chemical model in use involved the gas-dynamic transport of a viscous gas and the detailed kinetics of hydrogen oxidation [10]. Equations were solved with the upwind, finite volume procedure. The Roe flux vector-splitting scheme with a min mod limiter was used for the discretization of the fluxes in the equations. In the all cases considered here, the solid surface was assumed non-catalytic and adiabatic. The time step was 0.1 – 1 μs. The code was verified in work [7] against measurements in a shock tube.

In 2D case computational domain represented a quarter of a circle of the radius 20-50 mm. Number of cells was N = 100x100x50. Minimum space step was 0.1x0.1 mm^2, maximum - 0.3x0.3 mm^2. Boundary conditions are shown in Figure 1 (left).

In 3D case computational domain represented a quarter of a cylinder. The radius was 10-15 mm, the generatrix was 20-30 mm. Number of cells was N = 50x50x100. Minimum space step was 0.1x0.1x0.1 mm^3, maximum - 0.5x0.5x0.7 mm^3. Boundary conditions are shown in Figure 1 (right).

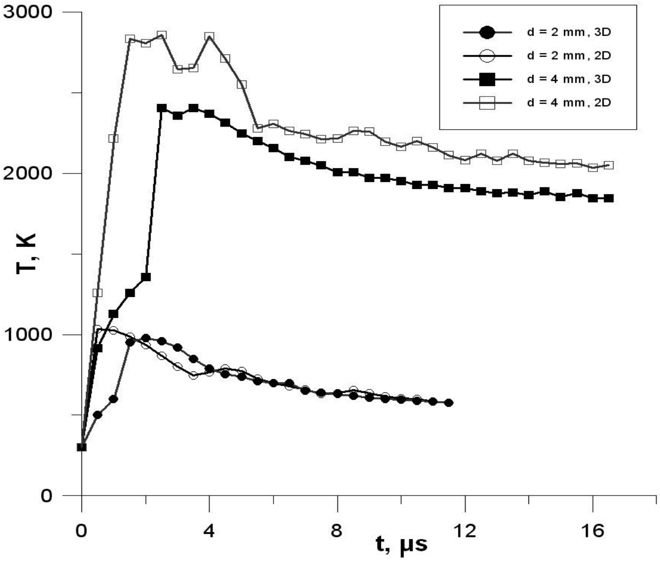

Figure 2. Maximum jet temperature vs. time. Initial pressure was 400 atm. Circles – orifice of 2 mm in diameter. Quads – 4 mm in diameter. Empty quads and circle correspond to calculations in 2D case, filled ones - 3D case.

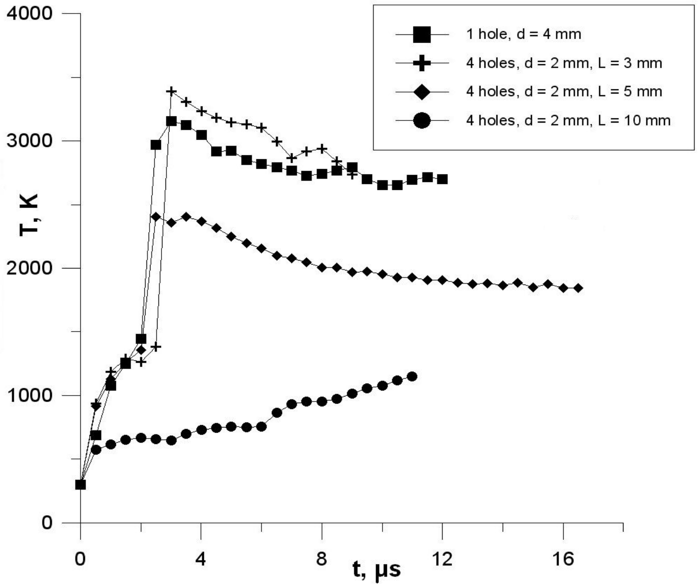

Figure 3. Maximum jet temperature vs. time. Initial pressure was 400 atm. Quads – 1 hole, D = 4 mm. Crosses – 4 holes, d = 2 mm, L = 3 mm. Rhombuses – 4 holes, d = 2 mm, L = 5 mm. Circles – 4 holes, d = 2 mm, L = 10 mm.

At first, test calculations were done for a single orifice of diameter 2 mm and 4 mm in 3D case. Initial pressure was 400 atm. The results were correlated with the data from 2D calculations, and with results from the work [9]. The reason to do the test calculations was to make sure that the use of a rather coarse grid in 3D does not result in big numerical error. In Figure 2. a comparison in maximum temperature of the hydrogen jet between two-dimensional and the dimensional cases for two different type of orifices is presented. Circles correspond to the orifice of 2 mm in diameter: empty circles – 2D case, filled circles – 3D case. Quads depict results for the orifice of 4 mm in diameter: empty quads – 2D case, filled quads – 3D case. Test investigation did not reveal any significant difference in the data obtained after 2 μs, the error being of the order of 10%. What was important that the general trend in temperature dependencies for the 3D case was conserved. Namely, ignition does occur for the orifice diameter 4 mm, but there is no ignition for the 2 mm orifice.

Finally, simulations were performed to reveal influence of the distance between orifices on diffusion self ignition. After replacement of the orifice with 4 mm diameter by area-equivalent system of 4 orifices with 2 mm diameter each, placed at 3 mm from each other, an increase in maximum jet temperature occurred. That can be explained with the interference of shock waves on the axis of symmetry. However, when the distance between orifices got long enough in comparison with the diameter – 10 mm, self-ignition did not occur.

4 Conclusion

In this work, an investigation of hydrogen jet at its release into atmosphere from a high pressure vessel was done. Results for several boundary and initial conditions have been compared. An optimum ratio between inlet orifices diameter and distance between them was obtained that was sufficient to depress diffusion self-ignition phenomenon.

References

[1] Breitung W. (2006). Mechanistic safety analysis of hydrogen based energy systems. Proc. 2nd European Summer School on Hydrogen Safety, Keynote Lectures, 2.

[2] Astbury GR, Hawksworth SJ. (2007). Spontaneous ignition of hydrogen leaks: A review of postulated mechanisms. Int. Journal of Hydrogen Energy, V. 32, N. 13, PP. 2178-2185.

[3] Wola'nski P, W'ojcicki S. (1973). Invest. into the mech. of the diffusion ignition of a combustible gas flowing into an oxidizing atmosphere. Proc. 14th Int. Symp. on Comb., PP. 1217 - 1223.

[4] Baev VK, Buzukov AA, Shumskii VV. (2000). Conditions of selfignition at impulse high pressure injection of combustible gases in confined volume. Combustion and Explosion. V. 36. N. 3. P. 3-9.

[5] Mogi T, Shiina H, Kim D, Horigushi S. (2006). Ignition of high pressure hydrogen by a rapid discharge. In Proc of The 31st Int. Symp. on Comb. Heilderberg, Germany.

[6] Dryer F, Chaos M, Zhao Zh, Stein J, Alpert J, Homer Ch. (2007). Spontaneous ignition of pressurized release of hydrogen and natural gas into air. Comb. Sci and Tech., 179: 663-694.

[7] Golub VV, Baklanov DI, Bazhenova TV, Bragin MV, Golovastov SV, Ivanov MF, Volodin VV. (2007) Shock-induced ignition of hydrogen gas during accidental or technical opening of high-pressure tanks. Journal of Loss Prevention in the Process Industries. V. 20. N. 4-6. P. 439-446.

[8] Bazhenova TV, Bragin MV, Golub VV, Ivanov MF. (2006) .Self ignition of a fuel gas upon pulsed efflux into an oxidative medium. Technical Physics Letters, 32(3), 269-271.

[9] Miller JA, Bowman CI. (1989). Mechanism and modeling of nitrogen chemistry in combustion. Progress in Energy Combust. Sci. V.15.

[10] Baev V, Golovitchev V, Tretjakov P, and et al. (1985). Combustion in Supersonic Flow, NASA TM-77822 : March.