Institutions of the Russian Academy of Sciences
Joint Institute for High Temperatures RAS
Institute of Problems of Chemical Physics RAS

Kabardino-Balkarian State University

Physics of Extreme States of Matter — 2010

Chernogolovka, 2010

Physics of Extreme States of Matter — 2010

Edited by academician Fortov V. E., Karamurzov B. S., Temrokov A. I., Efremov V. P., Khishchenko K. V., Sultanov V. G., Levashov P. R., Kanel G. I., Iosilevski I. L., Milyavskiy V. V., Mintsev V. B., Petrov O. F., Savintsev A. P., Shpatakovskaya G. V.

This compendium is devoted to investigations in the fields of thermal physics of extreme states of matter and physics of high energy densities. Different models and results of theoretical calculations of equations of state of matter at high pressure and temperature, physics of shock and detonation waves, experimental methods of diagnostics of ultrafast processes, interaction of intense laser, x-ray and microwave radiation, powerful ion and electron beams with matter, techniques of intense energy fluxes generation, low-temperature plasma physics, issues of physics and power engineering, and technology projects are considered. The majority of the works has been presented at the XXV International Conference on Equations of State for Matter (March 1–6, 2010, Elbrus, Kabardino-Balkaria, Russia). The edition is intended for specialists in physical and technical problems of power engineering.

The conference is sponsored by the Russian Academy of Sciences and the Russian Foundation for Basic Research (grant No. 10-02-06043).

ISBN 978-5-901675-96-0

© Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 2010

M.F., Laskin I.N., Saveliev A.S., Semin N.V., Volodin V.V. // J. Lost Prevent. Process Industr. 2008. V. 21(2). P. 185–198.
4. Gelfand B.E., Popov O.E., Chayvanov B.B. // Hydrogen: parameters of combustion and explosion (in Russian). M.: 2008. P. 288.
5. Sakurai A. // Proc. 15th Shock Waves and Shock Tubes Symposium 1985. P. 77–86.
6. Matthews C. // A quick guide to pressure relief valves (PRVs). Professional Engineering Publishing. London. 2004.
7. Divakov O.G., Eremin A.V., Ziborov V.S. // CD-Proc. 22nd Int. Symp. Shock Waves. 1999. Paper # 3974.
8. Bozhenkov S.A., Starikovskaia S.M., Starikovskii A.Yu. // 17th Int. Symposium on Gas Kinetics. 2002. CP. 25.

THE EFFECT OF BURST DISK OPENING ON COMBUSTIBLE MIXTURE FORMATION PRECEEDING HYDROGEN SPONTANEOUS IGNITION

Bragin M.V.*, Molkov V.V.

University of Ulster, Newtownabbey, United Kingdom (Great Britain)

**mv.bragin@ulster.ac.uk*

Abstract. Up to date little research has been done to study the effect of a finite time burst disk rupture on the formation of combustible mixture and spontaneous ignition of hydrogen during sudden release into air. An experimental observation of spontaneous hydrogen ignition at storage pressures as low as 13.5 bar was reported recently [1]. The paper investigates the difference in dynamics of the initial stage after opening of an imaginary non-inertial membrane and realistic inertial burst disk separating high pressure hydrogen from the air within a pressure relief device (PRD). The numerical simulations performed by the LES model.

Introduction. Hydrogen is an ecologically clean fuel to be used as an energy carrier or storage for renewable sources. Safety is the main concern for the emerging hydrogen economy.

It is known that sudden release of high-pressure hydrogen into air can spontaneously ignite without any apparent ignition sources present [2]. However, no references to spontaneous ignition problem or engineering design to avoid it can be found in regulations, codes and standards for handling compressed hydrogen.

Earlier numerical studies by Bazhenova et al. [3, 4], Liu et al. [5], and Xu et al. [6] were focused on unconfined release from high-pressure storage directly into the atmosphere. While spontaneous ignition was demonstrated by numerical simulations, no experimental proof exists up to date. Experimentally spontaneous ignition was observed in experiments with attachment tubes positioned downstream of a membrane by Dryer et al. [7], Mogi et al. [8, 9], Golub et al. [10, 11], and Pinto et al. [12]. The most recent study by Lenkevich et al. [1] demonstrated spontaneous ignition in a T–shaped pressure relief device (PRD) for initial hydrogen pressure as low as 13.5 atm.

In their earlier work Dryer et al. [7] speculated on the importance of the initial stage of membrane rupture on the mixing and subsequent spontaneous ignition process. They concluded that at low pressures, the chemical ignition time becomes the limiting factor, while at high pressures, the mixing time to achieve significant flammable mixture volume is the limiting factor. Up to now a little research have been done on this subject except recent works by Wen et al. [13] and Lee and Jeung [14] where the problem was partially addressed. The aim of this work is a comparative study of the initial dynamics of hydrogen-air mixing in the geometry of the pressure relief device (PRD) [1] for two cases: non-inertial membrane and inertial burst disk.

The model. The LES model of spontaneous ignition described in [15] is applied in this study. The set of main governing equations can be found elsewhere [16]. The RNG theory is employed for subgrid-scale modelling of turbulence. The reaction rate that appears in species transport equation was modelled using the Eddy-Dissipation-Concept (EDC) model [17], which incorporates detailed Arrhenius chemical kinetics. The model assumes that reaction occurs in small turbulent structures, called fine scales. In this study the detailed 21–step chemical reaction mechanism of hydrogen combustion in air employing 37 elementary reactions is applied [18].

Numerical details and burst disk rupture modelling approach. The geometry of high pressure system and T-shape PRD was taken from [1]. The high pressure system consisted of a 210 mm long tube with 16 mm internal diameter (ID) followed by a 280 mm long tube with 10 mm ID at the end of which the burst disk followed by a PRD was installed. PRD had 6.5 mm ID main tube with a flat end having two side openings connected to exit tubes of 4 mm ID.

The grid was created using GAMBIT tool of commercial CFD package FLUENT. The main tube and exit tubes were meshed with an unstructured hexahedral grid with uniform control volume (CV) size of about 400 μm both along the tube and a similar characteristic CV size in the cross-section. The anticipated combustion area was meshed with tetrahedral CVs with size of about 200 μm. The high-pressure chamber was meshed with the smallest CV size of about 250 μm clustered near the entrance to the simulated tube/low-pressure chamber and rapidly increasing away from it reaching the maximum cell width of 10 mm at the far end. The total number of control volumes was equal to 417.685.

Following [19], the rupture time of the diaphragm was calculated using equation (1), where ρ is the density of the diaphragm material (8900 kg/m^3 for annealed copper), b and d are the thickness (50 μm) and the diameter of the diaphragm (6.5 mm), respectively,

© Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 2010

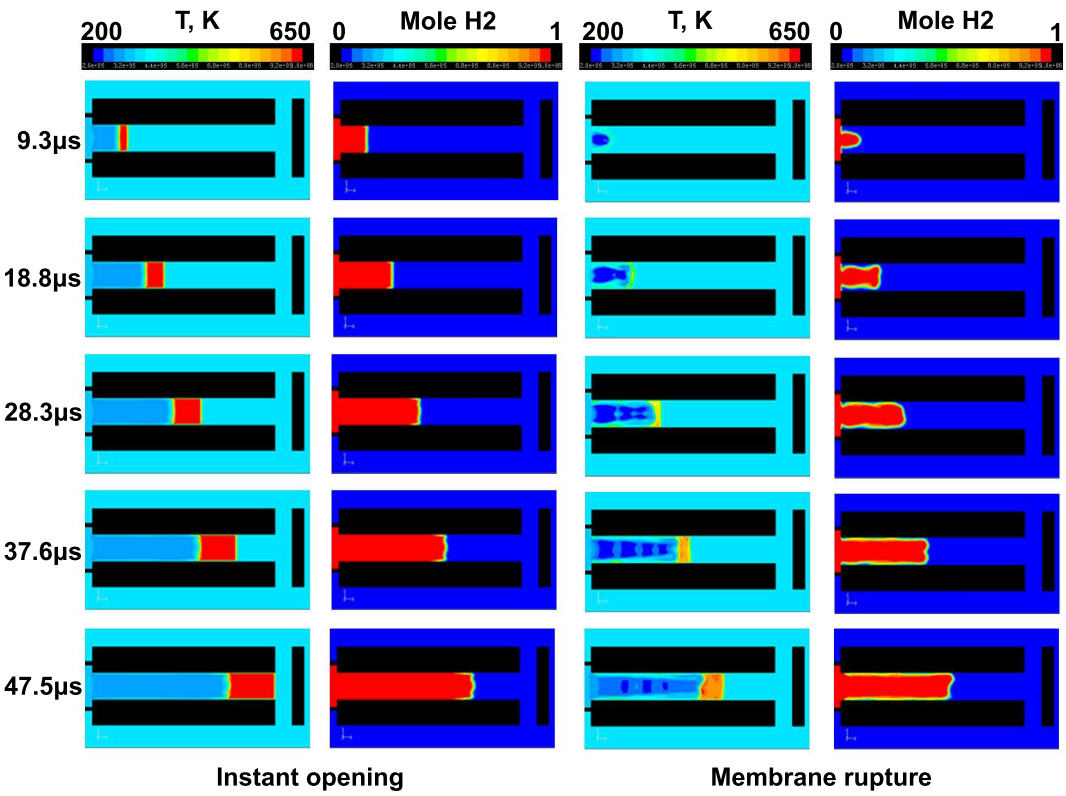

Figure 1. Comparison of temperature and mole hydrogen concentration dynamics for instant opening (left) and membrane rupture (right).

the value of k is 0.92, pressure p is taken as 13.5 atm.

$$t = k\left(\frac{\rho b d}{p}\right)^{\frac{1}{2}} = 0.92 \times \left(\frac{8900\ 5\ 10^{-5}\ 6.5\ 10^{-3}}{1.37\ 10^{6}}\right)^{\frac{1}{2}} = 42.3\ \mu\text{s}. \quad (1)$$

The burst-disk rupture process was approximated by 10 concentric rings openings in a step-like manner with opening times of each section listed in Table 1.

Table 1. Opening time of sections for 13.5 bar release.

Section	1	2	3	4	5	6	7	8	9	10
Time, μs	0	4.7	9.4	14.1	18.8	23.5	28.2	32.9	37.6	42.3

Non-slip impermeable adiabatic boundary conditions were used on all walls. The high pressure system was modelled as closed to exclude potential effects of numerical boundary conditions on the process. This assumption is applicable because the observation time in simulation is less than a time required for rarefaction wave to reach the end of high-pressure system. Initial conditions for high-pressure system were $p_0 = 13.5$ atm, $T_0 = 300$ K and the mole fraction of hydrogen equal to 1. Low pressure chamber was filled with air (0.23 mass fraction of oxygen and 0.77 of nitrogen) at $p_0 = 1$ atm and $T_0 = 300$ K.

The problem was simulated using general-purpose CFD package FLUENT 6.3.26, which realises control-volume based finite-difference method. The solver used explicit linearisation of the governing equations with explicit method for solution of linear equation set. A second order upwind scheme with AUSM flux splitting was applied for flow discretisation. The four step Runge-Kutta algorithm was employed for advancement of solution in time. The time step was determined from Courant-Friedrichs-Lewy condition, where the CFL number was equal to 0.2 to ensure stability.

Results and discussion. Figure 1 presents the dynamics of temperature and hydrogen mole fraction in the initial stage after hydrogen releases into air. The membrane rupture process is governed by the formation of under-expanded jet from the membrane with increasing in time open fraction of the tube cross section. A barrel-like structure can be seen. The opening of the next concentric ring of the burst disk generates barrel of larger diameter and the flow pattern looks similar to the diamond-like shapes. For the case of instant opening of the non-inertial membrane the shock heated zone is almost three times thicker compared to the inertial membrane rupture case at the same moment of time. The inertial opening of the membrane generates more mixing between hydrogen and air, especially in the boundary layer of the tube walls. Maximum temperature in the shock-heated air is 50 K lower for the case of inertial membrane opening.

Conclusions. The initial dynamics of temperature and mixing of hydrogen with air in the PRD main tube following the burst disk rupture is studied. The comparison of membrane and instant openings of a burst disk was carried out. It was shown that for the case

© Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 2010

of instant opening, shock heated zone is almost three times thicker compared to the inertial membrane rupture case at the same moment of time. The inertial opening of the membrane generates more mixing, especially in the tube wall boundary layer. Maximum temperature in the shock-heated air is 50 K lower for the inertial membrane opening case. Shock wave propagates faster for the non-inertial membrane.

1. Lenkevich D. A., Volodin V. V., Golub V. V. et al. // Proc. FLUCOME10, Moscow, 17–21 August, 2009.
2. Wolanski P., Wojcicki S. // Proc. Comb. Inst. 1972. V. 14. P. 1217.
3. Bazhenova T. V., Bragin M. V., Golub V. V. et al. // Proc. 25 ISSW, 17–24 July, 2005, Bangalore.
4. Bazhenova T. V., Bragin M. V., Golub V. V. et al. // Tech. Ph. Let. 2006. V. 32. P. 269.
5. Liu Y.-F., Tsuboi N., Sato H. et al. // Proc. 20 ICDERS, 31 July–5 August 2005, Montreal.
6. Xu B. P., El Hima L., Wen J. X. et al. // J. Loss Prev. Proc. Ind. 2008. V. 21. P. 205.
7. Dryer F. L., Chaos M., Zhao Z. et al. // Comb. Sci. Tech. 2007. V. 179. P. 663.
8. Mogi T., Shina H., Kim D. et al. // W–i–P poster 31 Int. Symp. Comb. 6–11 August 2006, Heidelberg.
9. Mogi T., Kim D., Shina H. et al. // J. Loss Prev. Proc. Ind. 2008. V. 21. P. 199.
10. Golub V. V., Baklanov D. I., Bazhenova T. V. et al. // J. Loss Prev. Proc. Ind. 2007. V. 20. P. 439.
11. Golub V. V., Baklanov D. I., Golovastov S. V. et al. // J. Loss Prev. Proc. Ind. 2008. V. 21. P. 185.
12. Pinto D., Aizawa K., Liu Y. F. et al. // Proc. 21 ICDERS, 23–27 July 2007, Poitiers.
13. Wen J. X., Xu B. P., Tam .Y. // Comb. Flame. 2009. V. 156. P. 2173.
14. Lee B. J., Jeung I. –S. // Int. J. Hyd. En. 2009. V. 34. P. 8763.
15. Bragin M., Molkov V. // Proc. 3 ICHS, 16–18 September 2009, Ajaccio. Paper 265.
16. Molkov V., Makarov D., Schneider H. // J. Phys. D: App. Phys. 2006. V. 39. P. 4366.
17. Magnussen B. F. // Proc. 19 AIAA, 12–15 January 1981, St. Louis.
18. Gutheil E., Balakrishnan G. and Williams F. A. // Reduced kinetic mechanisms for applications in combustion systems / Eds. Peters N., Rogg B. New York: Springer–Verlag, 1993. P. 179.
19. Spence D. A., Woods B. A. // J. Fl. Mech. 1964. V. 19. P. 161.

FLAME EVOLUTION WITHIN CLOSED VOLUMES

Ivanov M.F., Kiverin A.D.*, Rikov Yu.V.

JIHT RAS, Moscow, MIPT, Dolgoprudny, Russia

**alexeykiverin@gmail.com*

Introduction. Combustion gasdynamics within confined volumes studying is a basis for the optimum fuel combustion regimes design. The optimality is necessary when engine combustor or other energy-producing technical system is elaborating. It defines permanent interest in gaseous combustion within channels and tubes. A number of studies [1–3] concern flames propogating within opened and semi-opened channels. It allowed to gave a sufficiently detailed analysis of Darrieus-Landau (DL) instability—the leading factor defining laminar flame evolution.

It is principle point that patterns of DL-instability evolution obtained in studies with different boundary conditions prescribed on channel walls are rather different. Thus, in case of gas slip boundary conditions on the walls one can observe instability stabilization in time, the process becomes stationary and the flame front takes the quasi single-mode form [1]. In case of no-slip boundary conditions a highly perturbed wrinkled flame structure is formed, the flame front takes fornicated or tulip-shaped forms [2]. No-slip condition seems to be more natural because it is in agreement with molecular-kinetic theory results for gas interaction with solid surfaces. However experimental photos of gas mixture combustion in channels indicate existence of both quasi single-mode [4] and fornicated/tulip-shaped flames [5]. Accounting for the same mechanism of gas-surface interaction for most gases one can assume that in the real situation the flame front evolution depends on the specific combustible mixture composition not only quantitatively but qualitatively as well. In addition distinctions have to be observed for different channel widths [6, 7] and in presence of obstacles [6, 8].

The chambers walls are natural obstacles. Therefore flame dynamics within fully closed channel is distinct from dynamics within opened and semi-opened channels. It is defined by more complex combination of physical processes. Equally with intrinsic instabilities flame front is affected by acoustic waves generated by propagating flame itself and repeatedly reflected from the channel walls. In this case flame propagates in conditions of upwind flows and permanently growing pressure due to energy release within closed volume. Combined influence of flame instability and acoustic perturbations creates sufficiently complex evolution of the flame front propagating through the channel.

This paper represents numerical investigation of flame propagation in channels on the basis of hydrogen bearing combustible mixtures as an example. The comparative analysis of flame propagation in semi-opened and fully closed channels of different widths and lengths was carried out. Channels were filled with hydrogen-air or hydrogen-oxygen stoichiometric mixtures. No-slip conditions were prescribed on side walls of the channel. The numerical algorithm used is based on a mathematical model that describes the gas dynamics of real combustible mixtures in detail. Detailed model allowed to compare combustion dynamics in mixtures of different compositions [9].

Results. Analysis and discussion. Analyzing numerical modeling results (Fig. 1, 2) one can mark out three main stages of flame evolution in no-slip-walled channel. The first stage take place immedi-

© Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 2010