# NUMERICAL SIMULATION OF IGNITION OF HIGH PRESSURE HYDROGEN-OXYGEN MIXTURE JETTING TO ATMOSPHERE

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**الملخص**

أجريت محاكاة عددية لنفث لمخلوط الهيدروجين والأوكسجين تمت عملية تمدد عالية وذلك باستخدام برنامج (KIVA-3V) الذي يستخدم في حل المعادلات المضطربة ثلاثية الإبعاد والمصاحبة لها تفاعلات كيمائيه للغازات. وفي هذا التحليل استخدمت طريقة لاغرانج في حل طور الغاز لموجات الصدمة الناتجة من تمدد المخلوط .شكل الصدمة المتكونة من هذه العملية تم حلها عدديا أعلى فتحة النفث بمدى صغير.في هذه الورقة تم تحليل التمدد للنفث من ضغط عالي جدا ( 30 MPa) إلى ضغط الهواء الجوى لمخلوط الهيدروجين والأوكسجين وذلك باستخدام المحاكاة العددية المباشرة لفتحة صغيرة قطرها 2 مم خلال جدار الخزان. ونتيجة للاختلاف الكبير بين الضغطيين تتكون موجة الصدمة وبالتالي يتبعها تكوين الماخ القرصي الذي بدوره يعمل على تسخين المخلوط إلى حين الوصول للإشعال الذاتي للمخلوط. وتم في هذه الدراسة الحصول على معلومات قيمه ويمكن الاستفادة منها في معرفة سلوك النفث العالي خلال فتحات صغيره لخزانات الوقود ومعرفة تأثير قرص ماخ الناتج من التمدد العالي خلال جدران خزانات الوقود وبالتالي معرفة مقدار السلامة في عملية نقله وحفظه.

**ABSTRACT**

Numerical simulations have been carried out for highly under-expanded jet from an accidental release of high-pressure hydrogen–oxygen mixture into the atmospheric pressure by using KIVA-3V software. The original KIVA-3V [1] solves 3-D unsteady transport equations of a turbulent, and the chemically reactive mixture of gases. The gas phase solution procedure is based on a finite volume method called ALE (Arbitrary Lagrangian-Eulerian) method. A shock structure from the under-expansion is numerically resolved in a small computational domain above the jet exit. In this paper the investigate of a high pressure jet (30 MPa) of hydrogen-oxygen mixture by using a directed numerical simulation have been conducted. A small hole of 2 mm is assumed to be opened on the wall of a tank and a chocked mixture is injected to air. The autoigniton of pressurized hydrogen-oxygen mixture was predicted to first take place downstream of the Mach dick as the mixture heated to self-ignition temperature. Such knowledge is valuable for studying the ignition characteristics of high-pressure hydrogen jets in the safety context.

**KEYWORDS:** Hydrogen-oxygen; Under-Expanded Jet; Mach Disk; Large Eddy Simulation

## INTRODUCTION

The combustion of fossil fuel is responsible for the majority of greenhouse gas emission and a significant fraction of pollutant emissions in the world. Hydrogen is one of the most promising substitutes of hydrocarbon fuels, due to the absence of carbon-

cased pollutants, the abundance of hydrogen in nature, and the ability to generate hydrogen from sustainable energy source. The low viscosity and small molecular size of hydrogen give it a greater propensity to leak than other common gaseous fuels. The auto ignition temperature of hydrogen is only 800 K. It also has a stronger chain branching in its chemical reaction and reacts rapidly at a location where the temperature exceeds 1000K, while for hydrocarbon fuels rapid reactions occur until temperature is greater than 1500K.Hydrogen is viewed as a possible energy carrier after fossil fuels exhaustion. As it is estimated [2], world's reserves of oil will be sufficient only for the next 40 - 50 years. Hence, the hydrogen together with renewable and/or nuclear energy sources needs to be given greater consideration, despite the existing drawbacks. The main disadvantages of hydrogen as the energy carrier are its physical properties, especially low density that demands highly pressurized or liquid hydrogen storage, wide range of flammability (4 – 78 % vol. [3]), detonability concentration in air (18 – 56% vol. [3] ) and low ignition energy (0,02 mJ [3]). The risk for pressurized hydrogen release to auto-ignition is of great safety concern. Historically, there were incidents where sudden releases of high hydrogen were ignited with no clearly identifiable ignition source [4].
The mechanism of diffusion ignition was first proposed by Wolanski and Wojciki [4].

Very recently, Dryer et al. [5] demonstrated diffusion ignition of compressed releases of hydrogen into air by experiments. The experiments were conducted by administrating rapid ruptures of burst disks under different release pressures and internal flow geometries downstream the disks. Auto ignition occurred for release pressures above 20 bar. It was found that flow geometry downstream of the burst disk has a strong influence on auto ignition especially for lower release pressures. In their experiments, the rupture of the burst disks resulted in multi-dimensional transient flows involving shock formation, reflection and interactions. It was speculated that the multi-dimensional shock-boundary and shock-shock interactions played a key role in producing short mixing time scales for the auto ignition to occur.

In a very recent paper, Golub et al. [6] numerically and experimentally investigated the shock-induced ignition of high-pressure hydrogen releases. Their numerical results revealed that the auto ignition of the jet release was related to the hole size and no combustion occurred for the hole diameter less than 2.6 mm. In their experiment, the high-pressure hydrogen was released through a tube of constant area into a large chamber. The minimum required release pressure for auto ignition to occur was found to be dependent on the tube length. As the length was increased, the minimum required pressure dropped.

Xu et al. [7] simulate numerically highly under-expanded hydrogen jet. The vessel pressure and temperature is set as 20 MPa and 300 K, respectively and the orifice diameter is 1 cm. The release pressure, temperature and velocity are 10.6 MPa, 251 K and 1020 m/s, respectively. LES is selected to model turbulence in this problem. A 45-degree slice domain with diameter of 50D and length of 80D is used. The second order accuracy is employed but it is changed locally to a first order upwind to avoid non-physical oscillations. The maximum Mach number and velocity are 9 and 2700 m/s respectively.

In spite of continuous development of computational codes scientific research is still necessary for codes evaluation. This paper is aimed at enriching the data of hydrogen ignition characteristics during high pressure releases.

## NUMERICAL METHODS

Numerical simulations were performed with KIV-3V code. The code was developed in Los Alamos National Laboratory for internal combustion engine modeling, the solver is based on ALE (Arbitrary Lagrangian-Euler) used for the models with moving meshes and unsteady flows. Any additional information about the solver is described in the reference reports [8,9].The detailed chemical reaction mechanism is constituted by 9 species ($H_2$, $O_2$, O, H, OH, $HO_2$, $H_2O_2$, $H_2O$, and $N_2$) and 18 elementary reactions (Petersen and Hanson 1998) [10]. The pressure of hydrogen-oxygen mixture at the jet exit is 30MPa and the temperature is 300 K. The mixture was injected through a jet of 2mm in diameter to the test section of 30 cm long and 22 cm in width as shown in Figure (1).The initial ambience is air at 0.1 MPa, 300 K, and at rest. The combustion chamber divided in to 264000 cells. A uniform grid size of dx = dy=0.5mm is accepted in the simulation because our grid size resolution study before the simulation shows that the coarse grid size gives lower temperature prediction. It is necessary and reasonable to use such small grid size to simulate high temperature hydrogen combustion.

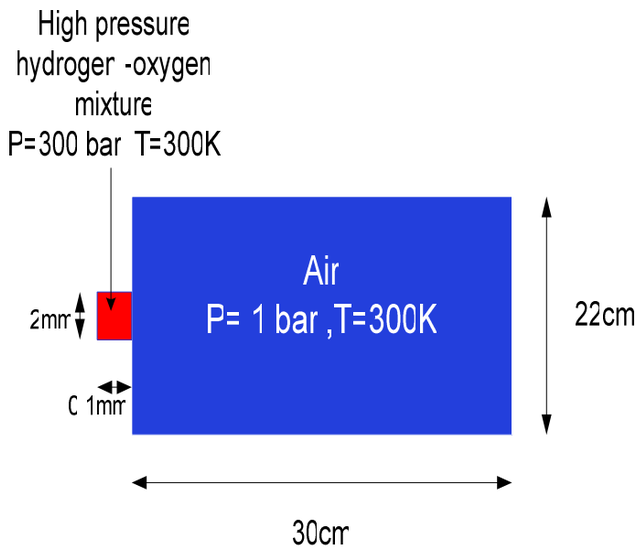


**Figure 1: The shape of the combustion chamber jet diameter.**

## RESULTS AND DISCUSSIONS

The Figure (2) shows main chamber pressure distributions for jet. The flow pattern of a jet issuing from the nozzle depends primarily on the pressure ration of the pressure at the nozzle exit to the ambient pressure. The first shock, which through the orifice, begins to diffract round corner .In next stage, a second shock which is generated in the vortex near the nozzle lip tends to spread toward the jet axis and finally to form a curved shock with an axe shape and Mack disk, The bow shock of a supersonic jet also forms where sonic disturbances generated along the trajectory converge .Highly under expanded jets, the subject of the present work, exit since $P_{jet}/P_a \approx 300$ and are characterized by the existence of multi shocks that are normal to the direction of the flow downstream of the flow downstream of the nozzle exit. The high expansion of the

$2H_2 + 0_2$ jet from 300 to 1 bars causes the pressure along its center line to become very low (less than 30 bars) relative to the ambient value (60 bars) and recompression takes place through a characteristic normal shock, or Mach disk. Immediately downstream of this first disk the flow is subsonic and the pressure increased to about 150 bars, although since supersonic flow persists in the surrounding region a slip line exists at the boundary of these two concentric domains. Since $P_{jet}/P_a$ is sufficiently high then the subsonic core of the jet is quickly accelerated and becomes supersonic once again so that a second Mach disk forms and the process begins all over again.

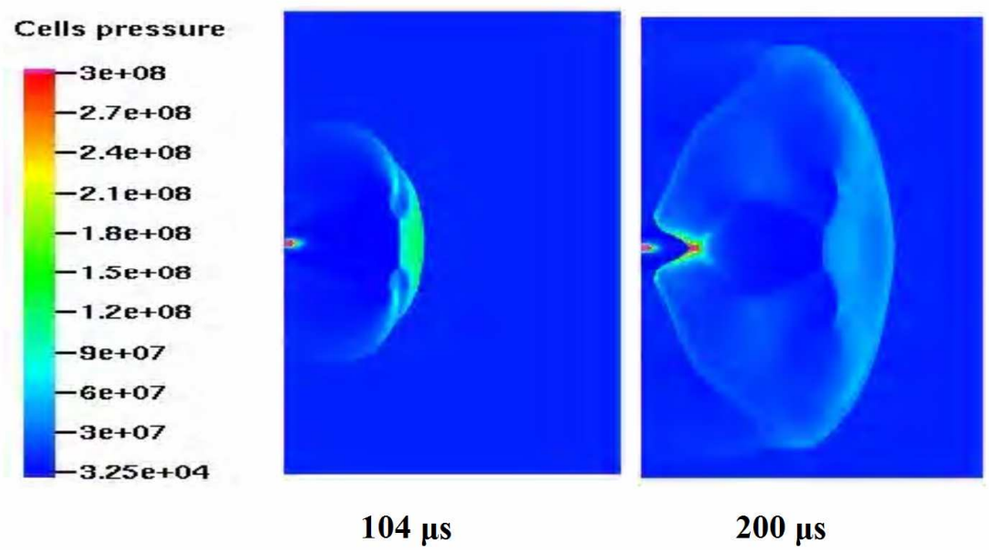


**Figure 2: Pressure contours at 104 µs and 200 µs.**

Figure (3) shows the temperature distributions at different moments in the combustion chamber for 2mm jet. As the $2H_2 + 0_2$expanded from 300 to 1bars, its temperature drops from 1300 K to 130 K. However, downstream of the first Mach disk it increases to about 1300 K and downstream of the second and third Mach disk the temperature increased to about 1170 K .If the temperature exceeds critical value, heat production dominates over heat flux to the surrounding. The temperature increases, which further accelerates the chemical reaction (chain branching) and results in growth of the radical concentrations, and thus, an explosion occurs. The ignition occurs at the tip of the jet downstream of third Mach disk after 128 µs from starting of injection and flame propagates sideways as results of expansion of high radicals concentrations (OH and $H_2O$) in the mixing zone to the ring vortex, and the final equilibrium temperature increased to 4380 K.

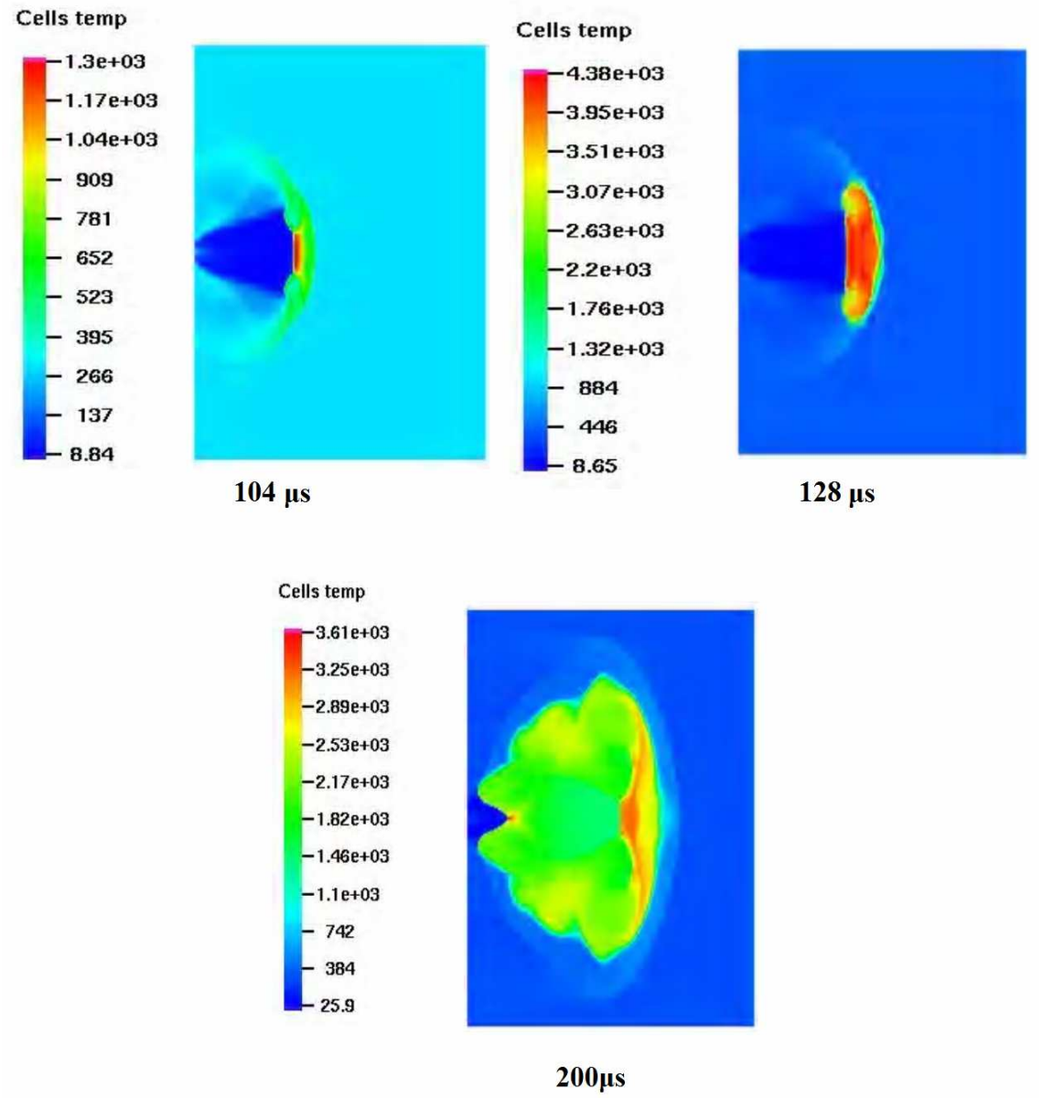


**Figure 3: Temperature contours at 104 µs, 128 µs and 200µs in 30 MPa tank pressure.**

The shock wave produced by stoichiometric hydrogen – oxygen mixture jet itself is simulated in order to study the mechanism of local combustion. The temperature contours are presented in Fig. 4; also the figure shows that the maximum temperature at the shock wave front at 80µs is higher than 888 K. This result demonstrates that the combustion at the contact surface is caused by the high temperature behind the shock wave.

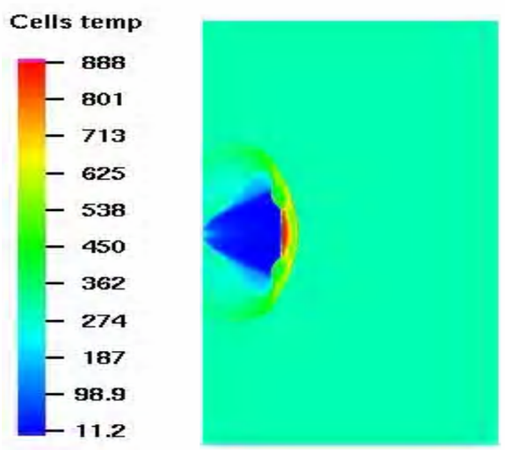


**Figure 4: Temperature contours of shock wave at 80μs in 30 MPa tank pressure.**

Figure (5) shows the mass fraction of OH, Figure (6) shows the mass fraction of $H_2O$ and Figure (7) shows the mass fraction of $H_2$ at 200 μs in 30 MPa tank pressure.

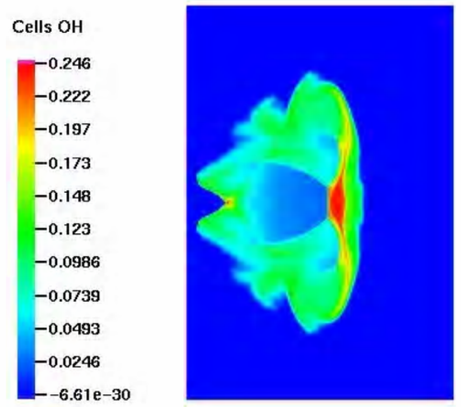


**Figure 5: OH mass fraction contours 200μs in 30 MPa tank pressure.**

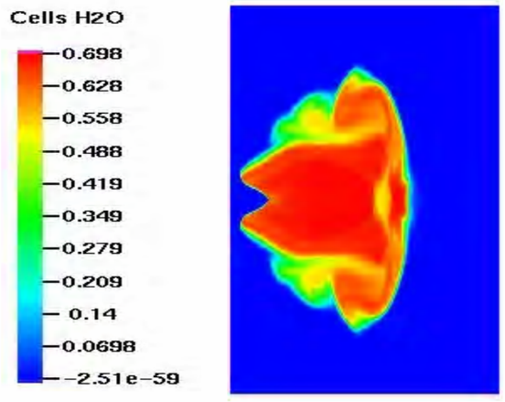


**Figure 6: Mass fraction contours of H2O at 200 μs in 30 MPa tank pressure.**

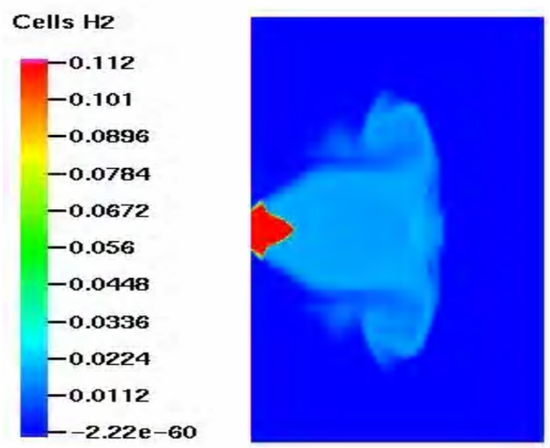


**Figure 7: Mass fraction contours of H2 at 200 µs in 30 MPa tank pressure.**

## CONCLUSIONS

Hydrogen-oxygen mixture release from a high pressure chamber is numerically simulated with computational fluid dynamics. A numerical simulation using Kiva3v-rel software have been successfully performed to predict the mixing and ignition of stoichiometric hydrogen-oxygen mixture jetting to air .Results of simulations have revealed that ignition of fuel-oxygen mixture starts after some delay in the zone of Mach disc at some distance from the jet exit. The time delay is required for mixing of hydrogen-oxygen mixture with air generate radicals and then ignition. After ignition flame propagates in both directions of the chamber. We investigate the behavior of a hydrogen-oxygen mixture jet coming into the air from 30 MPa high pressure tank by the direct simulation using two-dimensional Axisymmetric Euler equations with the full chemical mechanism, where the detailed chemical mechanism contains 9 species and 18 elementary reactions. Especially, the uniform grid size of dx = dy = 0.5 mm is used because our resolution study shows that the larger grid size influences the temperature at the jet front very much.

On the theoretical results of the study the following conclusions can be drawn:

- The local combustion of hydrogen-air mixture at the contact surface region occurs at the early stage of hydrogen-oxygen jet propagation. This local combustion is caused behind the shock wave induced by the high pressure hydrogen-oxygen jet. At 128 µs the local combustion increases the temperature at the contact surface up to 4,150 K.
- The time required to ignition the hydrogen - oxygen mixture jet is less than the time required to ignition hydrogen jet into the air, because high pressure hydrogen jet into the air needs time to mix first and after that ignition will start.
- The minimum ignition temperature is 1300 K and ignition start after 104 µs.

## REFERENCES

[1] Elhsnawi, M. and Teodorczyk, A. Warsaw University of Technology, ITC, Nowowiejska 21/25, 00-665 Warszawa, Poland. Experimental study of hot inert gas jet ignition of hydrogen-oxygen mixture

[2] Shafiee S., Topal E.: When will fossil fuel reserves be diminished? Energy Policy 37, 181-189, 2009.
[3] ADL. Arthur D. Little Inc. Final Report on an Investigation of Hazards Associated with the Storage and Handling of Liquid Hydrogen. Report C-61092, Cambridge, USA, 1960.
[4] Wolanski, P. and Wojcicki, S. (1972) Investigation into the Mechanism of the Diffusion Ignition of a Combustible Gas Flowing into an Oxidizing Atmosphere. Proc. Combust. Instit. 14, 1217–1223.
[5] Dryer, F.L., Chaos, M, Zhao Z. Stein, J.N., Alpert, J.Y. and Homer. C.J., Spontaneous Ignition of Pressurized Releases of Hydrogen and Natural Gas into Air, Combust. Sci. and Tech., 179:663-694,2007.
[6] Golub, V.V. , Baklanov, D.I. , Bazhenova, T.V. , Bragin, M.V. , Golovastov, S.V., Ivanov, M.F. , Volodin, V.V. (2007), Shock-induced ignition of hydrogen gas during accidental or technical opening of high-pressure tanks, Journal of Loss Prevention in the Process Industries, in press, available on-line.
[7] B.P. Xu , J. P. Zhang , J. X. Wen , S. Dembele , J. Karwatzki, Numerical study of a higly under-expanded hydrogen jet. Paper presented at the International Conference on Hydrogen Safety, Pisa, Italy, 8-10 September 2005.
[8] Amsden, A. A., O'Rourke, P. J. and Butler, T. D., KIVA -2: A Computer Program for Chemically Reactive Flows with Sprays. Technical report LA -11560-MS, Los Alamos National Laboratory,May 1989.
[9] Hirt, C. W., Amsden, A. A., and Cook, J. L. J., Comput. Phys. 14, 227, 1974
[10] E. L. Petersen and R. K. Hanson 1999 "Reduced Kinetics Mechanisms for Ram Accelerator Combustion," J. Prop. and Power, 15 (4): 591-600.