# Virtual experiments about hydrogen explosions with linear propagation

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**Abstract.** The dangers associated with hydrogen mainly come from its wide flammability range, it's extremely fast burning rate (having much more aggressive explosive properties than methane gas) and the considerable amount of energy released when it burns or explode. The development of new applications that use hydrogen as clean energy is constantly increasing, thus, hydrogen can be used on a large scale. This paper presents the use of computational fluid dynamics techniques, regarding the linear propagation of the explosion of air and hydrogen mixture in closed spaces, the main purpose being the determination of the overpressures to which a test stand of this processes is subjected.

## 1 Introduction

The present paper presents a virtual experimental stand model that is used for the analysis of linear propagation of explosions caused by air-hydrogen mixtures, in order to improve the level of safety and health at work [1], specific to industrial applications endangered by hydrogen generated explosive atmospheres and for technologies that generates low emission energy. The shortage of fossil fuels and the dangers regarding climate changes makes the application of hydrogen in association with renewable energy sources an interesting solution.

Still, the safety of hydrogen in production phase and the later use on large scale remains a significant concern. Hydrogen has different properties regarding the comparison with methane gas, some of these properties can help to reduce the dangers of this gas use. In other words, hydrogen is much lighter than air and has very good floatability and will quickly disperse in an unconfined space. Nevertheless, hydrogen requires lower energies for ignition and the traditional attenuation methods that are used for natural gas rarely works in the case of hydrogen.

Looking toward the future economy that includes hydrogen, two major domains can be envisioned namely cars industry and other vehicles that use hydrogen as fuel in combustion engine and fuel cells providing heating and electricity to households. In the last years, computational fluid dynamics has been used to perform risk assessments, mainly in the oil and gas industry. Based on the prediction of consequences of a huge range of potential accident scenarios [2], a level or risk is then estimated.

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## 2 Hydrogen explosive properties

Hydrogen is considered an important new energy carrier, meaning it can store and deliver energy in a usable form. At a standard temperature and pressure (0°C and 1013 hPa), we can discover hydrogen in a gaseous form. It is odorless, colorless, tasteless, non-toxic and lighter than air. The stoichiometric fraction of the mixture air and hydrogen is 70.4 % volume fractions of air and 29.6 % volume fractions of hydrogen, and for the mixture of oxygen and hydrogen, the stoichiometric fraction is 66.66 % volume fractions of air and 33.33 % volume fractions of oxygen. Abundant on Earth as an element, hydrogen is present everywhere, representing 75 % mass fractions of 90 % volume of al matter. Being an energy carrier, hydrogen is not an energy source itself, it can only be produced from other energy sources such as fossil fuels, renewable sources or nuclear energy through various energy conversions processes. The exothermic combustion reaction with oxygen forms water (combustion heat 1.4 x 108 J/kg$^{-1}$) and no carbon greenhouse gases are emitted into the atmosphere during the combustion.

The energy content of hydrogen is 33.3 kWh/kg$^{-1}$ corresponding to 120 MJ/ kg$^{-1}$ (the lower thermal power value) and 39.4 kWh/kg$^{-1}$ corresponding to 142 MJ/kg$^{-1}$ (the higher thermal power value). The difference between the lower and higher calorific value is the molar enthalpy of the vaporization of water, which is 44.01 KJ/mol$^{-1}$. We can obtain a higher thermal power as a result of burning hydrogen in the process of steam production, while the lower thermal power is obtained when the produced water is condensed back into liquid.

Compared to other fuels such as methanol, gasoline, diesel or kerosene, it is obvious that hydrogen produces much more energy per weight unit than any other fuel (about three times that of gasoline, diesel or kerosene) and can be dangerous to handle. The flammability range is the highest for hydrogen, but as long as it remains in an area that is properly ventilated there will be no risk of reaching this flammability range.

Furthermore, hydrogen has an ignition temperature of 560° C, unlike gasoline, which has an ignition temperature of 280° C. Hydrogen ignites very easily and burns with a wide range of mixtures with oxygen or air, compared to any other fuel [3]. Compared to most hydrocarbons, we find that hydrogen has a large flammability range, from 4 % volume fractions (lower flammability limit) up to 75 % volume fractions (upper flammability limit) in air, from 4 to 95 % volume fractions in oxygen and the detonation from 11 to 59 % volume fractions in air. These flammability limits increasing with temperature, for example the lower limit decreases from 4 % volume fractions at normal temperature and pressure (20°C and 1 atmosphere) to 3 % volume fractions at 100° C. Referring to these values, hydrogen has a very low minimum ignition energy of 0.017 MJ in air and 0.0012 MJ in oxygen at 25°C and 1 bar pressure. Regarding a comparison, the minimum ignition energy for most fuels is the range of 0.1 – 0.3 MJ, and for the oxygen they are at least an order of magnitude smaller.

Due to its low density, hydrogen do not accumulate near the ground, but dissipates into air, unlike gasoline and diesel. The comparative analysis of the risks in the event of an accident in closed and ventilates spaces, shows that both hydrogen and methanol are safer than gasoline, but in certain situations, hydrogen may present a greater risk than methanol.

As a short reminder regarding hydrogen explosive properties, we find that hydrogen can be initiated with ease in the presence of an ignition source, such as a spark, or a flame and even a surface with high temperature. Once initiated, hydrogen burns with an invisible flame, producing ultraviolet light. Also, hydrogen burns extremely fast and has a rapid flame expansion.

## 3 Linear design of virtual experimental stand used in data collection

In order to highlight the behavior of the linear propagation of explosions caused by the air-hydrogen mixtures in enclosed space, a computer simulation was carried out. The geometry of the linear stand was designed at a scale of 1:1 considering the following constructive parameters, in the table below:

**Table 1.** Constructive parameters of the linear virtual stand.

| Chambers | Dimension | Volume |
|---|---|---|
| Chamber 1 | 42.5 mm | 65750 $mm^3$ |
| Chamber 2 | 52.5 mm | 82750 $mm^3$ |
| Chamber 3 | 72.5 mm | 112750 $mm^3$ |
| Chamber 4 | 105 mm | 161500 $mm^3$ |
| Chamber 5 | 120 mm | 184000 $mm^3$ |
| Chamber 6 | 140 mm | 214000 $mm^3$ |
| Chamber 7 | 190 mm | 356500 $mm^3$ |
| Chamber 8 | 235 mm | 356500 $mm^3$ |
| Chamber 9 | 245 mm | 371500 $mm^3$ |
| Chamber 10 | 102.5 mm | 155750 $mm^3$ |
| Total length | 1350 mm | |
| Chamber sections | 50 x 30 mm | |
| Obstacle free sections | 40 x 20 mm | |

Since the computer simulation is based exclusively on the fluid medium, we get a total volume of the linear stand of 0.01199349 $m^3$. The virtual geometry of the linear stand design is represented in the figure 1.

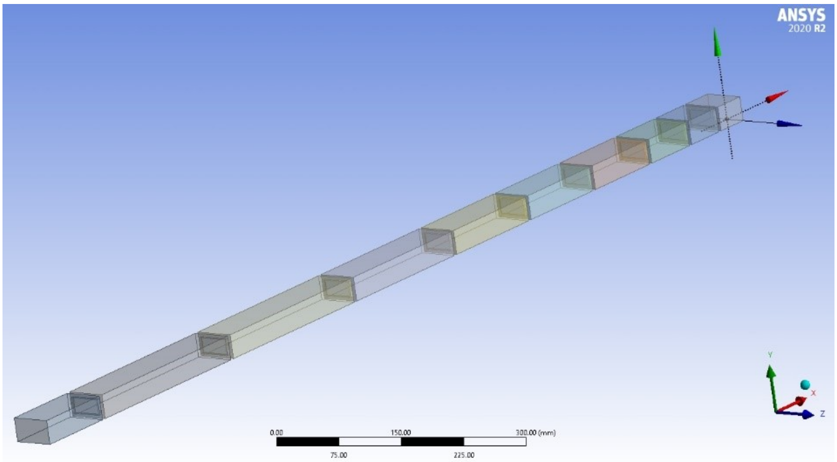

**Fig. 1.** Virtual geometry of the linear stand

The mathematical model used implements the method of finite volumes, so the resulting volume was divided (discretized) into 623493 calculation cells (finite volumes) necessary for running the algorithm. The computational cells are of different sizes, with the discretization mesh being more refined, with an element size of 2 mm, in areas of interest, such as the location of the virtual source if ignition of the air-hydrogen mixture, this being chamber number 1. The discretization network is shown in the figure below, figure 2.

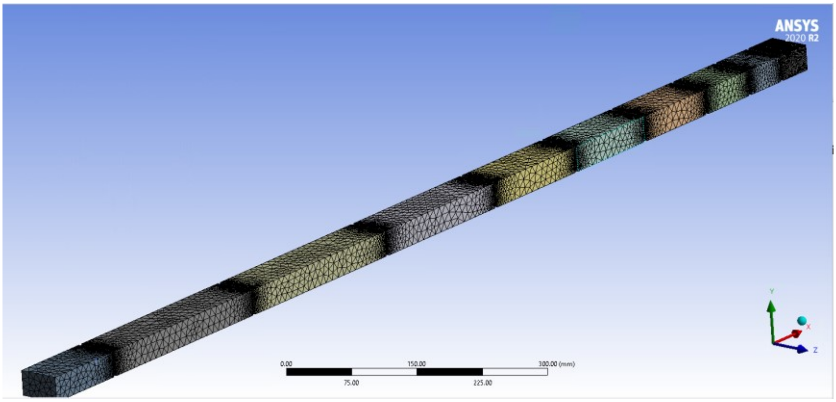

**Fig. 2.** Discretization of the volume of the linear stand in finite volumes

### 3.1 Input values used in the algorithm of FLUENT application

The fluid volume inside was set to a normal pressure of 101325 Pa with a temperature of 293 K (19.83°C), filled with air at 20.9 % volume fractions of oxygen, and the entire domain was set for ideal gas, compressible. The calculation algorithm was based on pressure, with a transient model. The contact surfaces between the chambers, are set as Mesh Interfaces as a common boundary.

The outer face of chamber 10 was set as surface outlet and initialized as pressure at 101325 Pa and 293 K (19.83°C). The chamber 1, 2, 3 and 4 have been set at a 20 % volume fractions of hydrogen in air. The initiation spark was placed inside the 1 chamber in the middle of the cross section and 15 mm from the closed end of the stand. In order to obtain results, reports of maximum pressure inside each chamber were defined [4].

## 4 Simulation results

Following the calculation process, a series of images were obtained representing the evolution of the flame front of the explosion regarding the air-hydrogen mixture, inside the linear stand. The images above represent the color contours of the pressure values recorded during the explosion process.

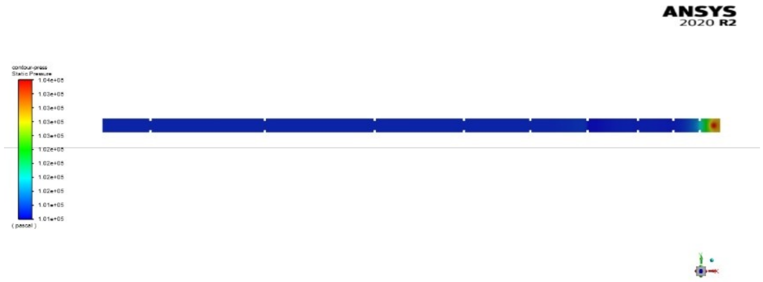

**Fig. 3.** Initiation of the explosive mixture air-hydrogen

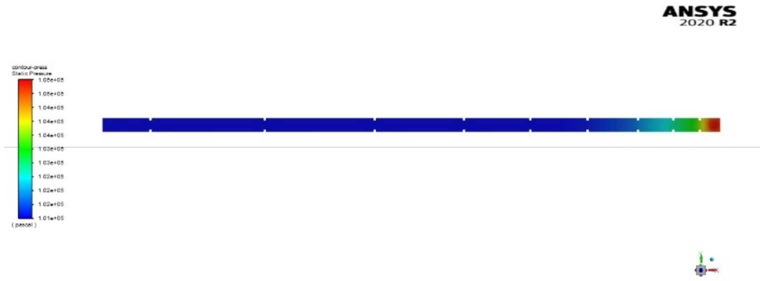

**Fig. 4.** Development of the explosion through the chambers

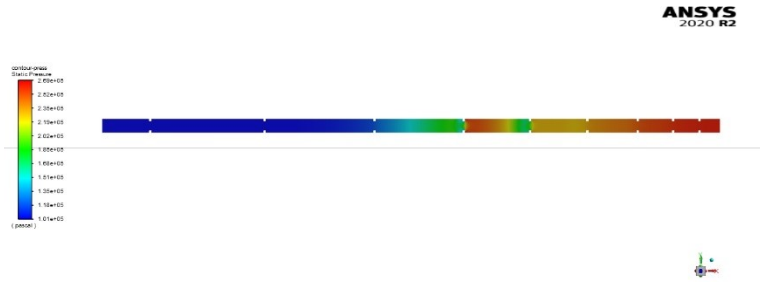

**Fig. 5.** The explosion front reaching chamber 7

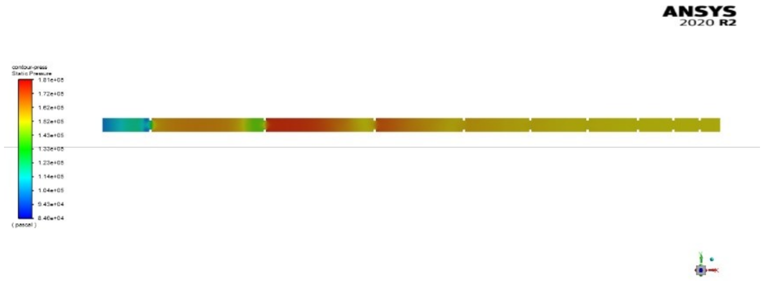

**Fig. 6.** Inclusion of the entire linear stand in the explosion process

At the end of the simulation, the maximum values of the absolute pressures in all 10 chambers are obtained. These maximum values are not necessarily those of direct waves passing over the sensor, they may be the result of reflected or combined pressure waves.

**Table 2.** Results obtained from the computer simulation.

| Chamber | Maximum Pressure (Pascals) |
|---|---|
| Chamber 1 | 268811.1054 |
| Chamber 2 | 270275.8606 |
| Chamber 3 | 295066.6518 |
| Chamber 4 | 359110.0445 |
| Chamber 5 | 355619.0681 |
| Chamber 6 | 269628.8026 |
| Chamber 7 | 223895.146 |
| Chamber 8 | 196894.7783 |
| Chamber 9 | 167098.1777 |
| Chamber 10 | 132051.4193 |

The table above with the maximum pressures is displayed in the figure below, figure 7.

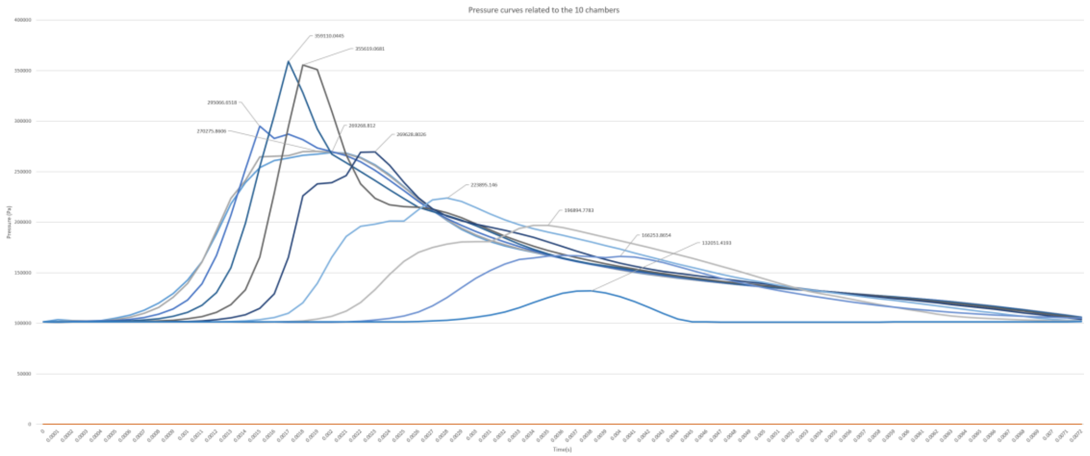

**Fig. 7.** Graphic display of the pressures recorded

# 5 Conclusions

As for conclusion, we can observe that the maximum pressure recorded was in the 4th chamber, increasing from the 1st chamber to 4th, the movement of the pressure in the linear stand can be compared with the movement of a piston that cause a variation of the volume inside a chamber (the piston principle), and from the lack of combustible support, the explosion extinguish and pressure are dropping, as we can observe in the figure 7.

Even if the simulation is not validated by the comparison with a physical experiment, it helps in the design of a stand for the study of hydrogen explosions, bringing a point of reference in considering the pressure fields as the main criterion in the choice of materials and in the way of developing the stand, for safe use.

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# References

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