The role of CFD analysis in studying hydrogen explosions with flame propagation direction changes

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Abstract. This study focuses on the transition from physical experimentation to virtual simulation, using Computational Fluid Dynamics (CFD) to analyses hydrogen-air explosions conducted in a transparent, rectangular-spiral test stand. The test stand was specifically designed to guide the explosion process along a spiral trajectory with 90-degree turns, aiming to replicate complex flame propagation behavior in confined geometries. The inner volume of the spiral was divided by four thin-film diaphragms, creating four sequential combustion chambers. This configuration allowed for controlled initiation and propagation of the explosion, enabling detailed observation of flame front behavior and the measurement of overpressure and flame speed across chamber transitions. The CFD analysis serves a dual purpose, to compare the explosion parameters obtained through virtual simulation with those recorded in physical experiments, and to calibrate the empirical input values required by the ANSYS Fluent solver for accurately modelling chain-reaction explosions in geometries with directional changes. The study emphasizes the importance of CFD in understanding flame dynamics in complex configurations, supporting both safety analysis and predictive modelling in hydrogen-related applications.

1 Introduction

In the current context of accelerated technological development and stringent requirements for safety and control in industrial processes, research into gas mixing systems is gaining particular relevance. These systems are essential components in leading industries such as chemical, biotechnological, pharmaceutical or semiconductor production, where the precision and reproducibility of gas mixtures directly determine the quality and safety of technological processes, Furthermore, the development of the system was based on mathematical models and control algorithms that allow fine-tuning of operating parameters, so as to respect the explosiveness limits within the spiral stand[1]. Comparatively, hydrogen does not present a greater inherent danger than other conventional fuels. As with the historical

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integration of other energy carriers, the establishment and enforcement of codes, standards, and safety procedures will be essential to ensure safe deployment and public acceptance. Under standard atmospheric conditions, hydrogen is a colorless, odorless, tasteless, and non-toxic diatomic gas. It undergoes liquefaction at a cryogenic temperature of −252.89°C. Being the lightest element, hydrogen has a very low volumetric density, approximately 14 times less than that of air. It exhibits high buoyancy and diffusivity, enabling rapid dispersion in open environments and permeation through minuscule apertures. These attributes complicate efficient storage and containment, and they also allow hydrogen atoms to diffuse into certain metals, particularly under high-pressure or high-temperature conditions, potentially causing hydrogen embrittlement, a degradation mechanism characterized by reduced ductility and strength of materials. Hydrogen exhibits favorable combustion characteristics, positioning it as a high-performance fuel. It possesses a specific energy (energy per unit mass) nearly three times bigger than that of gasoline. Its higher heating value (HHV) the total energy released upon complete combustion is also nearly threefold that of gasoline. Hydrogen allows combustion over a wide flammability range, typically between 4% and 74% by volume in air, and requires only a low minimum ignition energy. When oxidized either through combustion or electrochemical conversion (e.g., in fuel cells), hydrogen produces water vapor as the sole reaction byproduct, making it an environmentally favorable energy source. Despite these advantages, hydrogen's hazard potential arises from its physical properties. The primary acute risks associated with hydrogen leaks include fire, explosion, and asphyxiation [2]. In air, hydrogen forms flammable mixtures that can be ignited by thermal sources, open flames, electrical arcs, or electrostatic discharges. Hydrogen flames typically manifest as jet-like or torch-like plumes originating at the point of release, burning with high temperature and minimal radiant heat, and often being invisible to the human eye a condition that increases the likelihood of unintentional human exposure. Hydrogen's explosive potential is considerable, particularly in confined spaces, where a deflagration can rapidly transition to detonation due to the accumulation of pressure waves. Although the blast energy released by hydrogen explosions is generally lower than that of other fuels for the same energy content due to its rapid dispersion and low density the consequences can still be severe in enclosed environments. Moreover, although hydrogen is nontoxic, it can generate an asphyxiation hazard by displacing oxygen in poorly ventilated areas. However, such occurrences are rare, as the concentrations required to create oxygen deficient atmospheres typically fall within hydrogen's flammable limits thus, fire and explosion remain the principal hazards in hydrogen–air systems. In addition, liquid hydrogen (LH_2) introduces further risks due to its extreme cryogenic temperature, which can cause cold burns, material embrittlement, and cryogenic boiling hazards if not handled with specialized containment systems and thermal insulation.

1.1 Comparing hydrogen with other fuels

The table below provides a comparison of various fuel properties and characteristics for hydrogen, natural gas, gasoline, and propane.

Table 1. Hydrogen properties, natural gas, gasoline and propane.

	Hydrogen	**Natural Gas**	**Gasoline**	**Propane**
Lower heating value	119,957 kJ/kg	49,520 kJ/kg	41,860–44,220 kJ/kg	46,035 kJ/kg
Density at standard conditions	0.000084 kg/L	0.000599 kg/L	0.720–0.780 kg/L	0.506 kg/L
Phase at standard conditions	GAS	GAS	LIQUID	LIQUID

Autoignition temperature in air	566–582 °C	540 °C	257 °C	454–510 °C
Volume concentrations for flammability in air	4.1% – 74% volume	5.3% – 15% volume	1.4% – 7.6% volume	2.2% – 9.5% volume
Diffusion coefficient in air	0.610 cm²/s	0.160 cm²/s	0.052 cm²/s	0.110 cm²/s
Toxicity to humans	Non-toxic, simple, asphyxiant	Non-toxic, simple asphyxiant	Poisonous, carcinogenic. Irritant to lungs, stomach and skin	Non-toxic, simple asphyxiant

When evaluating hydrogen as both an energy carrier and fuel, it is essential to conduct a comparative analysis with conventional fuels. Hydrogen exhibits several inherent safety advantages over traditional hydrocarbons. Notably, certain combustion characteristics of hydrogen may render hydrogen related fires less hazardous than those involving conventional fuels. Due to its high flame propagation speed and rapid diffusivity, hydrogen whether in gaseous or liquid form tends to burn out quickly. Furthermore, the localized and high-temperature nature of hydrogen flames limits the ignition of adjacent materials, thereby reducing the likelihood of secondary fires, toxic smoke generation, and extended combustion durations.

2 Experimental model to analyze the development of air – hydrogen mixture explosions

In order to guarantee the optical components' alignment and stability and to allow access to the test section for the introduction of experimental setups or samples, the experimental stand's construction must be properly planned. To reduce measurement disruptions, other factors like environmental management (temperature and vibration, for example) could be required. Four interconnected chambers comprised a square spiral stand used for conducting physical tests on explosions of air-hydrogen mixtures. The building material for the experimental model used to assess the altered propagation of explosions was a polycarbonate sheet with a thickness of 20 mm [3]. The volume of this stand was divided into 4 separate chambers, as previously described, by 4 rectangular shutters made from two plates, each with two 12 mm diameter holes, with food-grade foil inserted between the plates. The volumes of the four chambers were, in order from the electrodes to the exit of the explosion tunnel, 150 cm³, 142.5 cm³, 207.5 cm³, and 1060 cm³. Compared to the tests carried out in the previous stage, this last volume, like the others, was sealed with a foiled shutter. The 4 pressure sensors were mounted at the shutter end of each chamber. The material polycarbonate was selected because of its great stress and pressure resistance as well as transparency. The inside portion of the explosion tunnel was established at 50 x 30 mm dimensions in consideration of the safety precautions for carrying out the experiments.
With this knowledge [4], the diameter of the parabolic reflectors used in Schlieren method recordings was the sole constraint. Consequently, a 50 mm wide by 20 mm wall spiral was built around the ignition chamber, which also contains the explosive mixture's source of initiation. This spiral continues until the end of a 412 mm-diameter circular section, as shown in figure 1. The spiral had an internal volume of 1.56 liters with a median line that measured 1040mm in length.

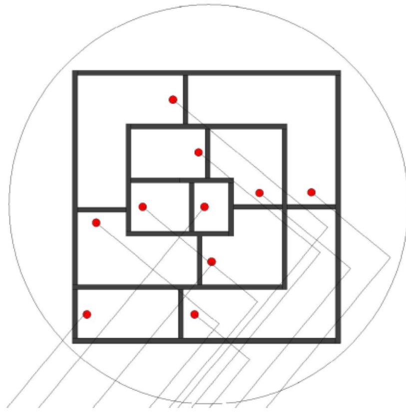


Fig. 1. Design of the spiral model used in physical experiments.

3 CFD analysis of hydrogen-air mixture explosion in experimental stand

The computerized simulation of the air–hydrogen mixture was carried out in two stages. The first stage focused on the explosion process and considered only the fluid volume of the prototype. Pressure values on the surfaces of the boundary walls were recorded, as well as the maximum overpressure value registered in the cells configured with explosive atmosphere. The membranes between the cells were removed (open surfaces), and the cells were defined only by the membrane support frames. The simulation [5] [6] was performed in ANSYS Fluent.

The second stage of the simulation involved importing the data obtained in the first stage, specifically the pressure values on the wall surfaces, and applying them to the surfaces of the solid bodies (the contact surfaces between fluids and solids) [7]. This simulation was performed in ANSYS Transient Structural [8] [9], and the virtual geometry of the spiral stand can be seen in figure 2.

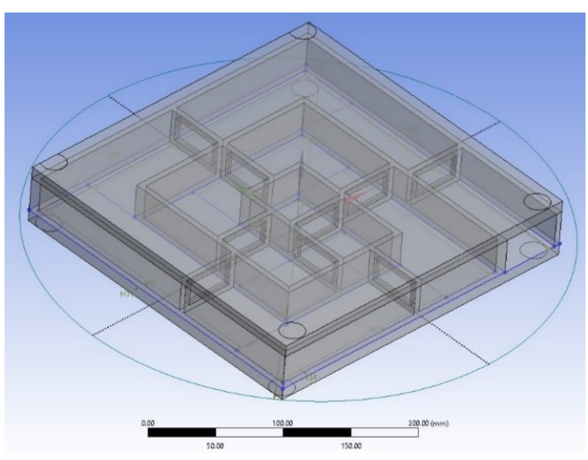


Fig. 2. Virtual geometry of designed experimental stand to test hydrogen-air mixture explosions.

3.1 First stage of analysis

Initial explosion settings in the fluid medium:

- Cells configured with explosive atmosphere: 1, 2, 3, and 4, starting with the central cell of the spiral;
- Hydrogen concentration in air: 20% volume fractions;
- Temperature: 20°C;
- Pressure: 101325 Pa;
- Ignition point: at the center of the spiral.

Results:

The maximum pressure recorded inside the volume of the spiral reaches a value of 351119 Pa, at t = 0.0044 s, peak captured in figure 3.

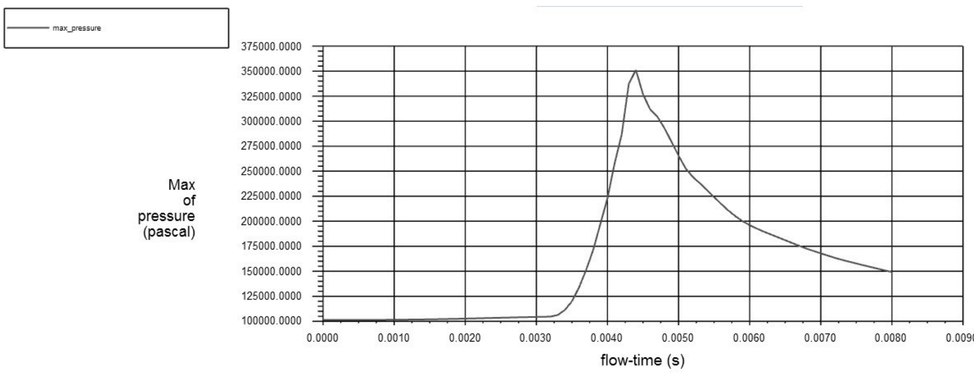
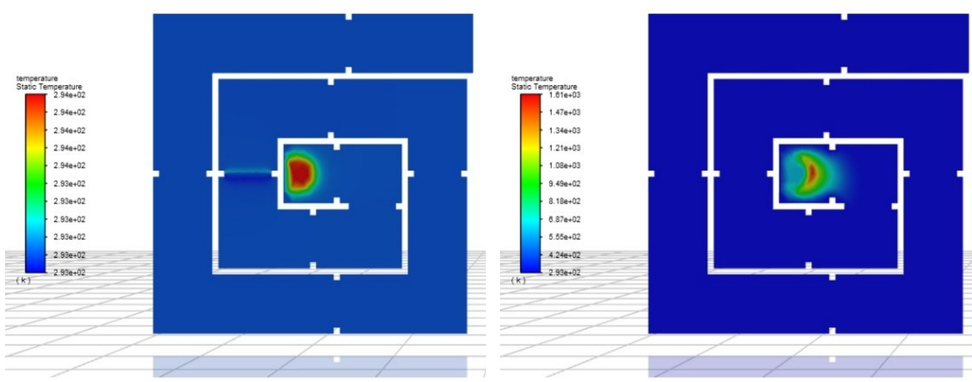


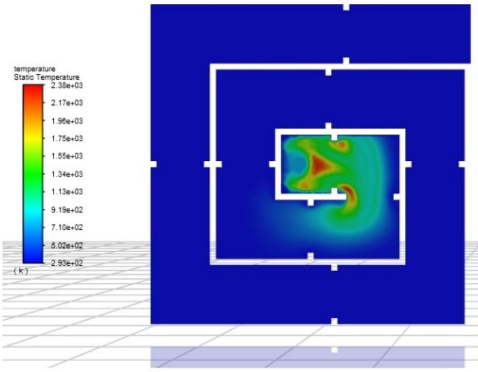
Fig. 3. The maximum pressure recorded inside the spiral stand

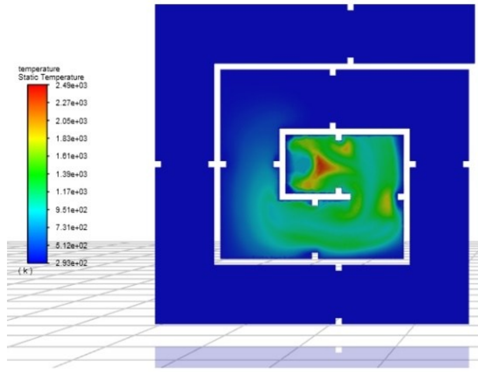
The behavior of the flame front, from the center of the spiral is represented through temperature contour plots, shown in the image sequence, figure 4 (from a to f):



a.) Starting point of explosion

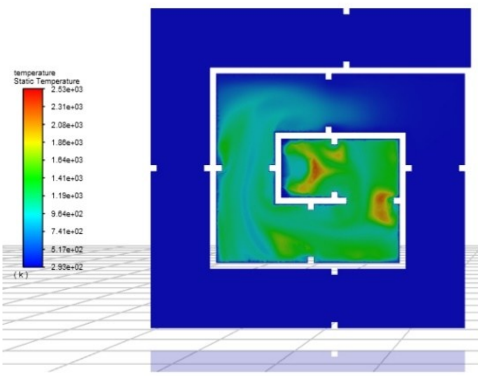
b.) Spiral centre flame propagation

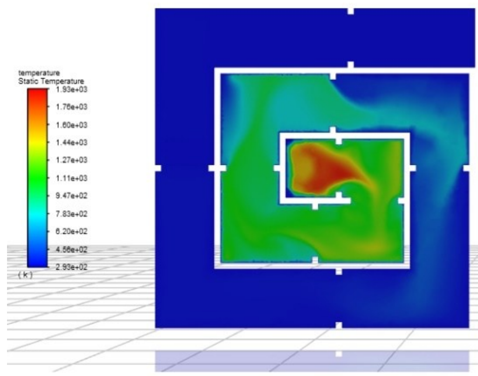




c.) Rapid evolution from the spiral centre

d.) Direction path of the explosion





e.) Modification of the explosion path

f.) Final evacuation of the flame front

Fig. 4. Sequence of images with color contours of temperatures

3.2 Second stage of analysis

The pressure values obtained in ANSYS Fluent during the first simulation stage, corresponding to the walls of the fluid volume—were transferred to ANSYS Transient Structural and applied to the solid bodies [10] [11] on the contact surfaces between them and the fluid volume (Figure 5). The top cover was intentionally hidden to allow visualization of the pressure application on the interior surfaces. The metallic spiral was assigned the Structural Steel material from the program's database.

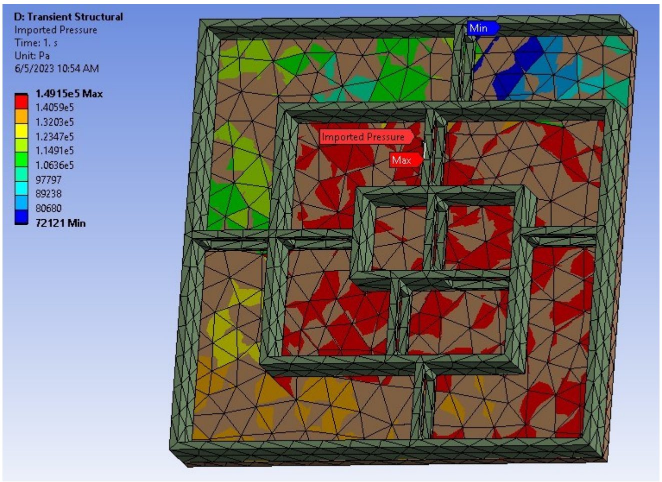


Fig. 5. Color contours of pressure values applied to the surfaces of solid bodies

The two plates—upper and lower—were defined with a thickness of 10 mm, having the following characteristics:

- Density: 1200 kg/m^3
- Ultimate tensile strength: 6E+07 Pa
- Yield strength: 5.5E+07 Pa
- Initial condition: Temperature: 20°C; Pressure: 101325 Pa;
- Boundary conditions: Fixed Support on four surfaces arranged in the corners of each plate

Results:

Following the ignition of the explosive mixture and the resulting pressure increase (as shown in the graph in Figure 3), the solid model exhibits a maximum deformation of 0.157 mm on the surface of the upper plate, at t = 0.0042 s (Figure 6).

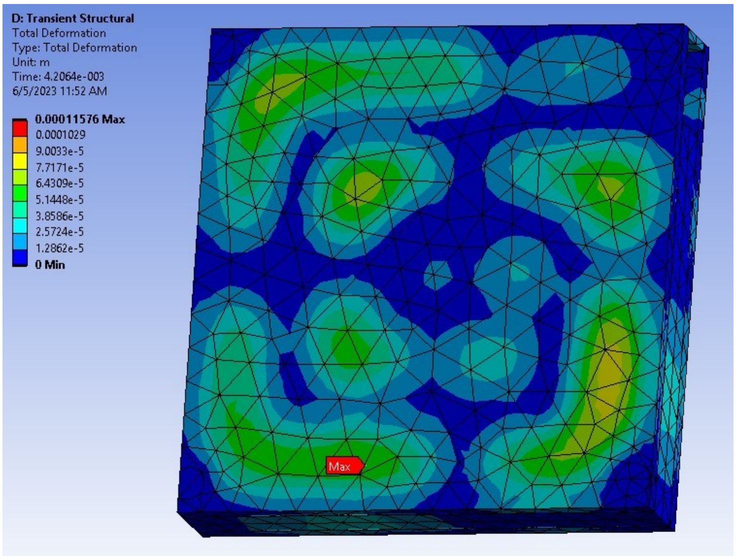


Fig. 6. Color contours of polycarbonate sheet deformations, with the maximum value highlighted

It should be noted that the computerized simulation presented at this stage of the project is intended as an approximation of the overpressure [12] values generated by the air–hydrogen explosion [13] [14] [15]. The results have not been validated through physical experiments conducted on the same geometry. Nevertheless, the set of obtained values offers the designer a useful reference point for dimensioning the polycarbonate plates and determining the assembly method for the experimental model.

4 Conclusions

The tests have successfully validated the functionality of the experimental model in terms of its ability to accurately record explosion pressures and effectively visualize and document the behavior of the flame front. This indicates the model's reliability for simulating and studying explosion dynamics. In summary, the conducted tests not only confirm the functionality of the experimental model but also reveal important nuances regarding the influence of directional changes and accidental gas leaks on explosion behaviors. These insights contribute to advancing both safety practices and scientific understanding in the field of explosion dynamics and mitigation.

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