Numerical Modelling as a Tool for Investigating Hydrogen Explosions

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Abstract

Currently, the burning of fossil fuels in industry or for transportation has a major negative impact on the environment. Most countries are concerned with environmental security and pollution regulation, motivating researchers around the world to find alternative solutions. An alternative solution may be the large-scale use of hydrogen. Applications of hydrogen in industry or for transportation face challenging conditions. Among other things, we are talking about pressures of up to 1000 bar, extreme temperatures starting from -253 °C (for liquefied hydrogen) and up to 650 °C - 950 °C (in the case of solid oxide electrolytic cells), as well as the imminent risk of explosion. This is because H2 has an extremely low ignition energy, with much wider flammability limits compared to other fuels such as methane or propane. Hydrogen is a highly reactive and explosive gas. Therefore, explosion protection is essential for all processes involving the use of hydrogen in one form or another. The same principles that are applied to natural gas can be applied. Hydrogen behaves similarly to methane in terms of explosion risk, meaning in principle that explosion protection works similarly for both gases. However, there are still many unknowns regarding the phenomenon of initiation and propagation of explosions caused by air-hydrogen mixtures. Taking into account the multiple aspects related to security techniques that must be taken into account for the use of hydrogen in industry or for transport, the current paper focuses on aspects with regard to the use of modern numerical modelling tools for increasing the occupational health and safety level in technological processes endangered by the occurrence of explosive atmospheres generated by air-hydrogen mixtures. It presents a review on the main research activities to be carried out within a the H2Model research project implemented between 2023 – 2026, project which focuses on numerical modelling on the ignition and propagation of explosions caused by air-hydrogen mixtures.

Keywords: numerical modelling, hydrogen explosions, air-hydrogen mixtures, enclosed spaces

Introduction

Currently, the burning of fossil fuels in industry or for transportation has a major negative impact on the environment. Most countries are concerned with environmental security and pollution regulation, motivating researchers around the world to find alternative solutions. An alternative solution may be the large-scale use of hydrogen.

Substantial decarbonisation is needed to meet the climate targets of the Paris Agreement in all greenhouse gas (GHG) emitting sectors. The transport sector tops this list and is one of the most difficult to decarbonise. Projections show that the amount of GHG reduction needed in the transportation industry between 2020 and 2030 is approximately 40 percent, 80 percent by 2050 [6]. Expecting an increase in transportation demand in the coming years, emission reductions / vehicle will should grow even more. In this sense, vehicles that use hydrogen as fuel to power their own propulsion systems should be used more than those that work on electric batteries, ensuring the transition of the transport industry to a "green" future.

However, environmentally friendly technologies must overcome a number of challenges, such as significant cost reductions, increased performance and an adequate infrastructure [2]. In addition, an important issue is safety in use.

Applications of hydrogen in industry or for transportation face challenging conditions. Among other things, we are talking about pressures of up to 1000 bar, extreme temperatures starting from -253 °C (for liquefied hydrogen) and up to 650 °C - 950 °C (in the case of solid oxide electrolytic cells), as well as the imminent risk of explosion. This is because H2 has an extremely low ignition energy, with much wider flammability limits compared to other fuels such as methane or propane [1], [3].

Hydrogen is a highly reactive and explosive gas. Therefore, explosion protection is essential for all processes involving the use of hydrogen in one form or another. The same principles that are applied to natural gas can be applied [4], [8], [16]. Hydrogen behaves similarly to methane in terms of explosion risk, meaning in principle that explosion protection works similarly for both gases.

However, there are still many unknowns regarding the phenomenon of initiation and propagation of explosions caused by air-hydrogen mixtures. The explosion limits of the air-hydrogen mixture are very wide. At the same time, air-hydrogen mixtures in the proportion of 17-60% detonate easily if they come into contact with an ignition source. In the case of detonation, the shock wave is very strong, the pressure reaching almost 20 times the initial pressure. If the shock wave encounters an obstacle, it can be reflected, the pressure increasing in this case up to 40 times [5], [12], [13].

At the international level, the use of computer simulations that support the research activity of events generated by explosions is relatively limited compared to the real danger that these events carry [15], [16], [17]. At the national level, the computer simulations carried out within INSEMEX, regarding the explosions of gas mixtures (mainly air - methane), are unique in Romania and of major importance in the prevention of these types of events. Thus, carrying out physical experiments and numerical modeling regarding the initiation and propagation of explosions of air-hydrogen mixtures, in the context of the use of this combustible gas as one of the main sources of energy, become imperative actions to prevent, in an intelligent manner, the effects produced by these phenomena [10], [11].

Research Aim

Considering the multiple safety engineering aspects that must be considered for the use of hydrogen in industry or for transportation, the overall objective of the H2Model project is to obtain input data sets suitable for precision computer simulations of chemical explosions of air-hydrogen mixtures in closed [14] and interconnected spaces and in open spaces, so that these modern tools can be used to increase the safety level in technological processes endangered by the occurrence of explosive atmospheres generated by air-hydrogen mixtures.

It is expected that the research presented will lead to the increase of the level of safety and health at work specific to industries endangered by explosive atmospheres generated by hydrogen, by designing and testing experimental models representing areas of analysis and study for the initiation and combustion of air-hydrogen mixtures, respectively by modeling numerical analysis of these phenomena in order to obtain input data sets suitable for precision computer simulations of chemical explosions of air-hydrogen mixtures in interconnected closed spaces and in open spaces [7], [9], [10].

Methodology and Results

The main objective of the research is to obtain input data sets suitable for precision computer simulations of chemical explosions of air-hydrogen mixtures in interconnected enclosed spaces and in open spaces. In this regard, the following results lay ground for achieving the target:

- obtaining a suitable data set for carrying out the simulations of hydrogen explosions in interconnected closed spaces, a tangible sub-objective by validating the results of the simulations through comparative analysis with the data recorded during the physical experiments;
- obtaining a data set suitable for the realization and validation of simulations of hydrogen explosions in open spaces, sub-objective achievable by comparative study of the results of the simulations carried out in the ANSYS FLUENT application with those obtained by using a software dedicated to this type of explosions (PHAST).

In the first instance, experimental models adapted to hydrogen explosions (much more aggressive than those of methane, butane or propane) are made, at the same time meeting the transparency requirements necessary for Schlieren recording techniques.

The second aim is to obtain approximately identical maps of overpressure values generated by hydrogen explosions in open spaces, by running two different applications (PHAST and FLUENT). Considering the fact that the PHAST application performs 2D simulations of this type of events [7], [9], the justification of the sub-objective is given by the virtual 3D representation of the phenomenon, through the FLUENT application both direct shock waves and reflected and combined ones are highlighted, the results being comparable with reality.

The following specific objectives are aimed out for achieving the target of research work:

a) development and instrumentation of experimental models;
b) testing the functionality of the experimental models used for the analysis of explosions caused by air-hydrogen mixtures in closed spaces;
c) physical experiments regarding the initiation of explosive air-hydrogen mixtures in closed spaces;
d) development of an experimental study aimed at the linear propagation of explosions caused by air-hydrogen mixtures in closed spaces;
e) experiments on the manifestation of explosions caused by air-hydrogen mixtures in closed spaces, as a result of the change in the direction of propagation;

f) transposition of experimental models in the virtual environment;
g) development of CFD simulations and their calibration in order to obtain sets of specific parameters suitable for use in CFD simulations of air-hydrogen explosions in closed spaces;
h) comparison of the results obtained through physical experiments with those obtained using CFD simulations;
i) use of specialized software for numerical modeling of discharge, dispersion in the atmosphere and explosion of hydrogen in open spaces;
j) transposition into the CFD model of the results obtained through the specialized software in order to obtain the sets of specific parameters suitable for use in CFD simulations of air-hydrogen explosions in open spaces;
k) case study on the applicability of the CFD model for the analysis of hydrogen explosions in open spaces.

Four phases are required for the proper implementation of the research work.

Conception, Development and Instrumentation of Experimental Models for the Analysis of Explosions Caused by Air-Hydrogen Mixtures

At this stage, two stands for experimenting with hydrogen explosions are made, with rectilinear propagation and, respectively, with a change in the direction of propagation. For this, are required:

- Identification of technical requirements and design of experimental models used for analysis of explosions of air-hydrogen mixtures: security parameters and design of experimental models are identified.
- Development and instrumentation of experimental models: experimental models with rectilinear propagation and with modification of the direction of propagation of explosions are developed.
- Testing the functionality of the experimental models: testing of initiation of air-hydrogen atmospheres, pressure recording and the applicability of Schlieren video recording techniques are performed.

Physical Experiments on The Initiation and Propagation of Explosions of Air-Hydrogen Mixtures

In this stage, a set of parameters of the explosions of air-hydrogen mixtures is acquired, regarding the initiation, rectilinear propagation and change of the propagation direction, through the following:

- Experiments regarding the initiation of air-hydrogen mixtures: the methods of initiation, by means of sources of different nature, of air-hydrogen atmospheres are investigated.
- Experiments on the linear propagation of explosions caused by air-hydrogen mixtures: the explosion parameters are obtained from physical experiments on the rectilinear propagation of explosions of air-hydrogen mixtures.
- Experiments on the development of explosions of air-hydrogen mixtures, with a change in the direction of propagation: the explosion parameters are obtained from physical experiments on the propagation of explosions of air-hydrogen mixtures with a change in direction.

CFD Modeling of the Formation and Initiation of Explosive Air-Hydrogen Mixtures Under Laboratory Conditions

In this step, a suitable input data set is obtained for performing computer simulations of hydrogen explosions in closed and interconnected spaces. This is achieved by:

- The transposition of the experimental models in the virtual environment: the virtual geometries of the real models in which the physical experiments of hydrogen explosions were performed and their meshing in finite volumes are realized.
- Realization of CFD simulations and calibration according to physical experiments: computer simulations are repeatedly run and the input data sets are modified to obtain conclusive results as close as possible to those from physical experiments.
- Verification and validation of CFD simulations: the results of computer simulations are accurately overlapped on those obtained from physical experiments.

Numerical Modeling of Hydrogen Explosions in Open Spaces

In this stage, the data is obtained from simulations of hydrogen explosions in open spaces, carried out with the help of a dedicated application, by:

- Numerical modeling of hydrogen discharge, atmospheric dispersion and explosion using specialized software for technological hazard analysis and consequence management in process industries: 2D simulations of hydrogen explosions are performed.
- Transposition into the CFD model of the results obtained through specialized software: a set of input data for CFD simulations, suitable for hydrogen explosions in open spaces, is finalized.
- Carrying out a case study on the applicability of the CFD model for the analysis of hydrogen explosions in open spaces: a comparative analysis of the effects of a hydrogen explosion produced in reality, in open space, with those obtained by computer simulations on the similar virtual geometric model is carried out.

Conclusion

The current paper represents a review on the activities carried out within H2Model research project for developing and testing experimental models adapted to hydrogen explosions (much more aggressive than those of methane, butane or propane), which also meet the transparency requirements necessary for Schlieren recording techniques. The final goal of numerical and experimental modeling is to obtain approximately identical maps of overpressure values generated by hydrogen explosions in open spaces, by running two different applications (PHAST and FLUENT). Considering the fact that the PHAST application performs 2D simulations of this type of events, the justification of the sub-objective is given by the virtual 3D representation of the phenomenon, through the FLUENT application both direct shock waves and reflected and combined ones are highlighted, the results being comparable with reality.

By completing and implementing the research results to be obtained obtained and considering the fact that computer simulations of hydrogen explosions belong to an insufficiently addressed field on a global and national level, it can be appreciated that there is expected a strong scientific impact, characterized mainly by:

- Increasing the degree of precision and, implicitly, increasing the quality of computer simulations of hydrogen explosions, by applying the new sets of input data obtained;
- Increasing the level of safety and health at work for technological processes endangered by the occurrence of explosive air-hydrogen atmospheres.

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