National University of Science and Technology
POLITEHNICA Bucharest

Doctoral School of Energy Engineering

Faculty of Power Engineering

DOCTORAL THESIS

Hydrogen – an Industrial and Energy Vector for the Transition to a Climate-Neutral Society

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Bucharest

2025

Abstract

The thesis entitled "Hydrogen – an industrial and energy vector for the transition towards a climate-neutral society" investigates the integrated use of hydrogen as an energy vector, with emphasis on the characteristics of combustion processes and on technological solutions compatible with this fuel. The work highlights the necessity of reassessing the physicochemical properties of the resulting gaseous fuels and of combustion equipment, in order to adapt to the challenges generated by the use of mixtures with high hydrogen content. The diffusion combustion technology was studied in detail, a technology that offers high combustion stability and allows the increase of the hydrogen proportion beyond the 15–20% limit currently achieved in premixed combustion with air. The research underlined the role of internal architecture and the need for precise control of operating parameters, particularly the air–fuel ratio. The architecture of the proposed system is completely innovative, thus providing an effective response to current challenges in the energy sector. The applied component of the research included the modeling and numerical simulation of a diffusion burner designed for the combustion of H_2–CH_4 mixtures with a hydrogen content of up to 50%. Using advanced computational fluid dynamics (CFD) methods in the ANSYS Fluent platform, issues related to flame stability, temperature distribution, and gas emissions were analyzed, with the aim of promoting low-carbon alternative fuels. The simulated model reproduces the operation of a burner under real industrial conditions, and the results obtained indicate optimal operating stabilities and validate the potential of using such gaseous fuel mixtures as a sustainable energy transition solution. The validation of the simulations was carried out through an experimental program developed using a specially designed test stand. This was equipped with the innovative burner and with advanced instrumentation for real-time monitoring of flow and combustion parameters, such as flame temperature, pressure, and gas flow rates. The separate feeding of hydrogen and methane allowed the preparation of variable mixtures, tested under controlled conditions, providing highly accurate experimental data useful for the optimization of diffusion combustion technology. Considering these aspects, the objective of the thesis is the detailed exploration of the effects of different proportions of hydrogen mixed with methane on the general characteristics of combustion, including flame stability, energy efficiency, and pollutant emission levels. Although previous studies have highlighted the significant influence of hydrogen on combustion processes—sometimes in contradiction with the behavior of methane - this thesis has clarified the exact mechanisms and complex interactions between the two fuels. By conducting an extensive set of experiments and analyzing flame behavior at different equivalence ratios, the thesis contributes to a deeper understanding of the gas-dynamic, thermodynamic, and kinetic phenomena involved. In this context, the thesis makes an important contribution to the specialized literature, opening new directions for future research in the field of alternative fuels and energy efficiency in the combustion of H_2–CH_4 mixtures.

Keywords: hydrogen energy vector, energy transition, diffusion combustion, diffusion burner, numerical simulation, experimental validation.

Preface

The thesis entitled "***Hydrogen – an Industrial and Energy Vector for the Transition towards a Climate-Neutral Society***" addresses the strategic role of hydrogen in the context of the energy and industrial transition, analyzing its potential to contribute to the decarbonization of economic sectors with high greenhouse gas emissions.

In the current context of climate change and increasing pressures to reduce carbon emissions, the research of alternatives to fossil fuels becomes essential. Hydrogen, as a clean fuel, has significant potential in the transition towards a low-emission economy. In particular, hydrogen mixtures with natural gases, such as methane, represent a valuable opportunity for the integration of hydrogen in the first stage of the energy transition, facilitating the optimization of combustion processes and the reduction of the ecological impact associated with the use of conventional fuels.

The main objective of the research includes the development of predictive models and combustion optimization strategies, intended for industrial applications, with emphasis both on thermal performance and ecological impact. These studies lead to innovative technological solutions in the field of energy and the reduction of polluting emissions, having a significant impact on the sustainability of industrial processes and the efficient use of resources.

The global energy transition, imposed by the necessity of reducing greenhouse gas emissions and adapting to new climatic realities, has opened the path towards a profound rethinking of energy production and utilization systems. In this context, hydrogen is increasingly asserting itself as a strategic energy vector, with extensive applicability in industry, transportation, and the generation of electric and thermal energy. However, its integration into a decarbonized energy mix requires a rigorous, multidisciplinary approach that addresses the technical, technological, and safety challenges associated with the use of this fuel.

The present work is part of this effort of knowledge and innovation, proposing a complex analysis of the behavior of hydrogen in combustion processes and developing concrete application solutions for its utilization in industrial and residential installations. By combining numerical modeling with experimental testing, the author provides a relevant contribution to the understanding of the combustion mechanisms of H_2–CH_4 mixtures and to the optimization of burner configurations compatible with these fuels.

Within the thesis, the research was carried out with high methodological rigor, using state-of-the-art simulation tools and a solid, scientifically grounded applied approach. The innovative architecture of the proposed system and the quality of the experimental results support the idea that hydrogen is not only a promise for the future, but also a real solution for the present, when supported by advanced research and precision engineering. This work is addressed not only to the academic community but also to specialists involved in the development of sustainable technologies for the energy sector. The thesis brings a significant contribution to the path towards a climate-neutral economy, combining applied research with theoretical research in a forward-looking vision.

In its development, the thesis addressed Chapter 1 "***Hydrogen – Energy Vector in Industry***", which establishes the essential role of hydrogen in the context of the energy transition, emphasizing its potential as a strategic vector in reducing carbon emissions. Its integration into fuel mixtures with methane allows the capitalization of existing infrastructure, facilitating the rapid decarbonization of industrial and energy sectors. Although protium is widely used in commercial applications, a deeper understanding of hydrogen's behavior requires the analysis of isotopic differences. These determine significant variations in properties such as diffusivity, thermal conductivity, and the kinetics of chemical reactions. In this respect, deuterium and tritium are becoming increasingly relevant in advanced research and the development of emerging nuclear technologies,

especially in the context of controlled fusion. In order to capture the current scientific maturity of the subject, a historical incursion into the evolution of knowledge of this element is necessary. From the empirical observations of the alchemists and the early experiments of Cavendish and Lavoisier, to modern uses in space propulsion, nuclear reactors, and quantum technologies, hydrogen has established itself as a key element of technological progress. The discovery of deuterium and tritium marked a paradigm shift in nuclear physics, opening new directions of research and strategic applications. The chapter details the fundamental characteristics of the three natural isotopes of hydrogen – protium (^{1}H), deuterium (^{2}H or D), and tritium (^{3}H or T) – highlighting the mass differences and their impact on performance in technological processes. The specific properties of each isotope, methods of production, as well as relevant applications in industry, energy, and scientific research are analyzed. The influence of these differences on the efficiency of combustion systems, the behavior of nuclear fuels, and numerical modeling in energy engineering is also emphasized. Deuterium is presented as a valuable tool for investigating reaction mechanisms and the functioning of heavy water reactors, while tritium is considered indispensable for the future success of nuclear fusion. The chapter explores the experimental and theoretical path of the discovery of these isotopes, including the essential contributions of scientists Urey, Aston, Rutherford, and Alvarez. Detection methods, safety implications, and critical applications within the ITER and DEMO projects are also analyzed. An extended section is dedicated to hydrogen isotope production and separation technologies. Established industrial methods such as steam methane reforming (SMR), partial oxidation, and autothermal reforming are presented, alongside sustainable alternatives such as water electrolysis or the exploitation of natural hydrogen sources. Advanced separation processes – cryogenic distillation, catalytic isotopic exchange (VPCE, LPCE, CECE), membrane permeation, thermal diffusion, and differential adsorption – are analyzed in detail. In this context, the contribution of research carried out at ICSI Râmnicu Vâlcea is highlighted, especially regarding the development of detritiation installations and separation infrastructure intended for the CANDU and ITER projects. The chapter also addresses the technological, economic, and safety aspects associated with hydrogen isotopes, including challenges related to isotopic selectivity, energy consumption, material compatibility, and contamination risks (especially in the case of tritium). Modern solutions for monitoring, protection, recovery, and regulation are discussed, as well as emerging research directions – artificial intelligence, new catalysts, and integration with renewable sources. Additional emphasis is placed on the importance of hydrogen purity in high-precision applications, analyzing refining methods such as pressure swing adsorption (PSA), thermal swing adsorption (TSA), separation with metal hydrides, and selective membranes. Finally, the industrial and energy applications of the isotopes are highlighted, consolidating the image of hydrogen as a multidisciplinary resource and a central element in the transformation of energy systems. Uses in CANDU reactors, nuclear fusion, energy storage, and the synthesis of special compounds reflect the strategic relevance of hydrogen in the transition towards a clean and sustainable economy. The structure of the chapter thus provides a solid conceptual framework for a thorough understanding of hydrogen and its isotopes, essential for the development of innovative technological solutions. Isotopic analysis is not only an academic concern, but a pillar of global strategies regarding climate neutrality, energy security, and the circular economy.

Chapter 2 "***Green Hydrogen – Energy Vector***" addresses, in an integrated and scientifically grounded manner, the issue of the transition towards a hydrogen-based economy, highlighting its essential role as a strategic energy vector in the decarbonization process of the energy system. Within the chapter, the main stages of the energy transition are analyzed, such as the increase in the share of renewable energy sources (RES), the development of carbon capture and utilization (CCU) technologies, and the importance of implementing Power-to-Gas (PtG) technologies for energy storage. Special attention is given to Power-to-X (PtX) systems, which allow the conversion of renewable electricity into green hydrogen, methane, or other synthetic fuels with wide applicability in industry, transport, and the residential sector. The chapter also includes a comparative analysis of the three major electrolysis technologies – alkaline (AEC), proton exchange membrane (PEM), and solid oxide (SOEC) – evaluating them from the perspective of energy efficiency, operational flexibility, technological

maturity, and implementation costs. Economic and technical aspects regarding the production of green hydrogen at the European scale are presented, highlighting the national and regional energy potential for the integration of these solutions. The possibilities of storage, transport, and interconnection of natural gas and hydrogen networks are also addressed, underlining the advantages of hybrid solutions for balancing electricity grids in the context of the increasing share of intermittent renewable sources. Moreover, the issues addressed in Chapter 2 provide a solid theoretical and applied basis for understanding the complexity of the energy transition and for identifying the strategic role that hydrogen can play in building a sustainable energy infrastructure. It is emphasized that future energy systems will increasingly integrate green hydrogen, not only as a storage vector but also as an efficient solution in transport and industry, through injection into the methane grid or use in dedicated installations. Power-to-X technologies are becoming essential tools for transforming renewable energy surpluses into useful fuels, contributing to grid stability and seasonal storage. Concrete examples, such as the 20HyGrid pilot projects in Romania and Green Hysland in Spain, confirm the feasibility of these solutions under real conditions. In this framework, the thesis proposes the development of a diffusive burner dedicated to the combustion of H_2–CH_4 mixtures, as part of predictive models for the optimization of combustion processes with reduced pollutant emissions, thus contributing to the consolidation of the technological basis necessary for the transition towards a sustainable economy.

Chapter 3, "***Technological Particularities of the Combustion of Gaseous Fuels, including Hydrogen–Methane for the Energy Transition***" is dedicated to the use of hydrogen and methane mixtures, examining in depth the technical and economic challenges associated with the integration of these solutions into the energy transition. Essential aspects such as the impact on existing infrastructure, operational safety, implementation costs, and environmental implications are analyzed, outlining a complex framework in which hydrogen can become a viable substitute for traditional fossil fuels, especially methane. Important emphasis is placed on the role of combustion technologies, which represent a critical link in the energetic utilization of hydrogen. In this regard, the thesis investigates the operating principles of gaseous fuel burners, presenting various configurations – premixed, diffusive flame, self-aspirating, and low-NOx emissions – and analyzing their applicability in real industrial contexts, including for the H_2–CH_4 fuel mixture. Based on a fundamental theoretical framework regarding combustion technology, the chapter details the behavior of turbulent jets, the interaction between fuel and air streams, as well as the criteria that determine flame stability and combustion process efficiency. It is emphasized that the adoption of hydrogen requires a profound re-evaluation of the physicochemical properties of gaseous fuels, the constructive configurations of burners, and combustion control strategies.

Chapter 4 "***CFD Simulation of a Diffusive Burner for Methane and Hydrogen Mixtures: Performances and Challenges***" investigates, through advanced numerical simulation, the behavior of a diffusive burner specially designed for the combustion of hydrogen and methane mixtures, with a content of up to 50% H_2 in the volume of the fuel mixture. The main objective of the research consists in the analysis of combustion processes – with emphasis on flame stability, temperature distribution, and emission formation – in order to promote low-carbon alternative fuels. The modeling was carried out in ANSYS Fluent, within a rigorous computational fluid dynamics (CFD) framework, applied to a detailed model of an industrial burner operating in controlled conditions. The study evaluates the combustion process performances for different compositions of the H_2–CH_4 mixture in stoichiometric, sub-stoichiometric, and excess air regimes, comparing the obtained results with those for the exclusive combustion of methane. The results obtained revealed optimal operating conditions and high flame stability, thus demonstrating the feasibility of the industrial use of hydrogen-rich mixtures. It is highlighted that diffusive combustion technology can support the safe and efficient burning of mixtures with up to 50% H_2, exceeding the usual limits of current applications carried out mainly for premixed combustion with air, which generally do not exceed 30% H_2 in the mixture. The research included, in the first part, the analysis of the flow distribution, followed by the investigation of the combustion process inside the burner, the characterization of the temperature field and the concentrations of reactive species (CO, CO_2, H_2O), as well as the

study of turbulent kinetic energy in the combustion zone. The conceptual architecture of the burner was patented. Numerical validation was performed based on a physical burner specially built and tested under controlled conditions on an experimental stand, which allowed the correlation of simulated data with the real behavior of the system. Through the integrated approach and high level of detail, the thesis makes a significant contribution to the understanding of the phenomenology of methane–hydrogen mixture combustion in diffusive regime and to the development of technological solutions for sustainable industrial applications. The conclusions of the research support the potential of burners adapted to alternative fuels to support the energy transition, ensuring both high thermal performances and the reduction of pollutant emissions. The data obtained can form the basis for the future development of predictive models and innovative technologies in the field of clean combustion.

The experimental research carried out is presented in Chapter 5 "***Experimental Research on the Combustion of the CH_4–H_2 Gas Mixture***", research that aimed at validating the numerical modeling applied to the diffusive burner specially designed for the combustion of hydrogen and methane mixtures, with a hydrogen content of up to 50%. The experimental stand built for this purpose was designed to simulate real operating conditions, allowing the acquisition of precise and relevant data, the stand as an original element constituting the subject of a registered patent. The pilot burner used is equipped with five nozzles for fuel supply, each nozzle being framed by a circular section for air intake, facilitating vertical combustion in free development regime. The measurements performed – temperature, pressure, flow rate, flame composition – highlighted a stable flame behavior, in agreement with the CFD predictions, demonstrating the efficiency of the constructive architecture. The results highlighted a progressive decrease of the flame velocity along the axial direction and complete combustion, without the formation of pollutants from CO or NOx above the limits specific to the fuel characteristics for regimes with controlled excess air ($\lambda \leq 1.3$). Also, through its concentric architecture, the stand allowed separate feeding with hydrogen and methane, offering flexibility and adaptability in configuring the H_2–CH_4 fuel mixtures obtained.

The validation of the numerical model through experimental data confirms the potential of H_2–CH_4 hybrid combustion in diffusive–turbulent regime, opening clear perspectives for efficient and sustainable industrial applications. The experimental stand and the tested burner provide a robust platform for further research on hydrogen combustion in various proportions and operating conditions. The conclusions of this research support the idea that the integration of hydrogen into the energy mix is not only technologically feasible, but also efficient in terms of performance and environmental protection.

The contributions of the thesis are detailed in Chapter 6 "***General Conclusions, Original Contributions, and Future Research Directions***", together with the general conclusions and future research perspectives.

Express of gratitude

The years of research dedicated to doctoral studies were full of challenges, sustained efforts to deepen my own knowledge, and the desire to contribute to the enrichment of scientific literature through the results of investigations carried out in a prestigious academic environment – the National University of Science and Technology POLITEHNICA Bucharest.

I express my deep gratitude to my supervisor, Professor Gheorghe LAZĂROIU, for the opportunity to develop myself and to carry out innovative research, as well as for the support offered in establishing remarkable collaborations. I also thank him for his role as a mentor in the academic and research environment, for his kind guidance, and for the constant motivation during these years of study.

Special thanks are addressed to Professor Lucian MIHĂESCU for the constructive comments, particularly useful observations, and the support provided in completing the doctoral thesis.

Last but not least, I wish to thank Professor Gabriel Paul NEGREANU and Professor Ionel PISA for the valuable discussions and advice offered during the progress meetings.

From the bottom of my heart, I want to thank the wonderful person who has been my unwavering support during this challenging period – my dear Honey – as well as my beloved daughters, Alexia and Alma, to whom I am deeply grateful for their understanding, calm, and priceless presence.

I am profoundly grateful to my parents, Elena and Alecu, for believing in me and supporting me unwaveringly.

I dedicate this research to my daughters, Alexia and Alma, whose love and smiles gave me the strength to move forward, with the message All our dreams can come true, if we have the courage to pursue them – **Walt Disney**.

The energy of the future is not found in material resources, but in the ingenuity and courage of scientists **– Nikola Tesla**

Chapter 1: Hydrogen – Energy Vector in Industry

1.1. Introduction

Hydrogen is emerging as an essential industrial vector in the context of the energy transition and clean technologies, due to its multiple role of transport, storage, and supply of energy in various applications, without direct pollutant emissions. The intensification of decarbonization policies and recent technological innovations have led to a substantial increase in interest in hydrogen, especially in strategic sectors such as transportation, heavy industry, and the residential sector. Through its versatility, hydrogen supports the restructuring of the energy and industrial system, contributing decisively to the reduction of greenhouse gas emissions. At the same time, the isotopes of hydrogen prove to be valuable resources for research and advanced applications, with relevance in nuclear energy, frontier medicine, and materials science, significantly broadening the horizon of this element's uses [1, 2].

1.2. Hydrogen - Brief History

The first observations of hydrogen date back to the 16th century, when Paracelsus described the appearance of a flammable gas resulting from the reaction between metals and acids. Later, Jan Baptist van Helmont introduced the term "gas" (1625), and Robert Boyle documented (1670) the production and combustion of a gas obtained from iron and sulfuric acid, a detail published in his 1672 work [3]. Nicolas Lemery confirmed the explosive character of the substance (1700). A major breakthrough was made by Henry Cavendish, who in 1766 isolated "flammable air" and described the formation of water through its combustion [4]. Antoine-Laurent Lavoisier identified hydrogen in 1783 as a distinct element, giving it its current name. In the same year, Jacques Charles launched the first hydrogen balloon, and Lavoisier and Laplace measured the heat of combustion. The 19th century brought the discovery of water electrolysis (Nicholson and Carlisle), the development of fuel cells (Schönbein and Grove), and cryogenic studies that led to the liquefaction and solidification of hydrogen (Wróblewski, Dewar). In modern physics, hydrogen played an essential role: the studies of Bohr, Schrödinger, and Pauli on the atom laid the foundations of quantum theory, while the discovery of its isotopes – deuterium (Urey, 1931) and tritium (Rutherford, 1934) – revolutionized nuclear research. The 20th century brought the use of liquid hydrogen as rocket fuel (1943), its use in thermonuclear tests (Ivy Mike, 1952), and the initiation of controlled fusion programs, from Tokamak (1956) to ITER (1985). This evolution, from the first empirical observations to applications in energy, physics, and industry, confirms hydrogen as a central element of scientific and technological progress, while its isotopes open promising perspectives for both fundamental and applied research.

1.3. The Importance of Hydrogen Isotopes in Industry and Theoretical Aspects of Separation

The isotopes of hydrogen – protium (^1H), deuterium (^2H or D), and tritium (^3H or T) – are fundamental in various industrial applications, from nuclear reactors to cooling technologies and spectroscopic analysis. Their different physicochemical properties give them specific uses, but their separation represents a technological challenge due to the very small differences in relative mass. At present, the main separation methods used in industry are cryogenic distillation, isotopic chemical exchange, and gaseous diffusion, each presenting its own advantages and limitations.

1.3.1. Protium, Deuterium and Tritium: Strategic Vectors in the Energy of the Future

Hydrogen, the lightest and most abundant element in the Universe, plays an essential role in the context of the energy transition, being considered a strategic energy vector for reducing carbon emissions. Its use in fuel mixtures, especially alongside methane, represents a viable solution for the decarbonization of industrial and energy sectors, without imposing significant modifications on the existing infrastructure. The combustion of hydrogen and methane mixtures thus contributes to the reduction of CO_2 emissions and to the diversification of energy sources with low environmental impact. Although in current commercial applications protium, the lightest and most stable isotope of hydrogen, is predominantly used, a deeper understanding of the behavior of this element requires the analysis of isotopic properties. Deuterium and tritium, the other two natural isotopes of hydrogen, present distinct physicochemical characteristics and are used differently depending on the requirements of technological processes. Hydrogen and its isotopes have relevant applications in the energy, chemical, and nuclear industries, each requiring specific methods of production, separation, and purification. In the context of the development of sustainable energy sources, the isotopes deuterium and tritium gain strategic importance, being considered essential fuels for future nuclear fusion reactors. This type of reaction, which imitates the natural processes inside stars, is emerging as one of the most promising technologies for obtaining a green, sustainable, and safe long-term energy source. Knowledge of isotopic differences is also essential in the characterization and optimization of advanced technological processes. Deuterium, in the form of heavy water, is used as a neutron moderator in CANDU-type nuclear reactors. Tritium is actively targeted in international nuclear fusion projects, such as ITER, due to its potential to generate high-yield energy reactions with almost zero pollutant emissions.

These applications highlight the fact that the isotopes of hydrogen are not just an academic extension of the study of elementary chemistry, but strategic tools for modern energy engineering. To fully understand the behavior and applicability of hydrogen isotopes, a comparative analysis of their fundamental physical and chemical properties is essential, as these directly influence performance in various industrial and scientific processes. In conclusion, the in-depth analysis of hydrogen isotopes – protium, deuterium, and tritium – represents an essential premise for the development of innovative technological solutions. These have direct applicability in the global energy transition, in the optimization of combustion processes of fuel mixtures, and in the development of next-generation nuclear technologies, with a significant impact on energy security and global sustainability.

1.3.2. General Properties of Hydrogen Isotopes

In nature, hydrogen exists in three isotopic forms: protium (^{1}H), deuterium (^{2}H or D), and tritium (^{3}H or T) [5]. Protium dominates current commercial and industrial applications, while deuterium and tritium are anticipated to play an essential role in the future of clean energy production, especially through the development of controlled nuclear fusion technologies. Protium (^{1}H) is the predominant isotope of hydrogen, representing ≈ 99.985% of natural abundance [6, 7]. At atmospheric pressure, it is found in gaseous form, becoming liquid at ≈ 20 K (–253 °C) and solid at ≈ 14 K (–259 °C) [8]. Deuterium and tritium are present in very small natural amounts and require specific processes to obtain usable quantities. They are used in scientific and industrial applications and represent the fuel for nuclear fusion reactors, a process considered to be one of the most promising alternatives for the sustainable production of green energy. Deuterium, the stable isotope of hydrogen, contains one neutron more than protium and has an atomic mass of 2.0141 u [7]. Although it represents only 0.0156% of natural hydrogen, this isotope has strategic importance in energy and scientific applications. Currently, deuterium has important applications in combustion research, being used as an isotopic tracer for investigating reaction mechanisms by controlled substitution of protium. Thus, it becomes a valuable tool in the analysis of rate-limiting steps in processes such as the combustion of methane–hydrogen mixtures. In addition, deuterium plays an essential role in the nuclear industry, being used in CANDU-type reactors, where heavy water (D_2O) acts as a neutron moderator [13, 14]. Tritium, symbolized as ^{3}H (or T), is the only naturally radioactive isotope of hydrogen, with a nucleus consisting of one proton and two neutrons, and a relative atomic mass of 3.016049 u [7]. The physical properties of the isotopes directly influence their performance in technological applications. Molecular diffusion is slower for deuterium and tritium, and thermal conductivity decreases with increasing isotopic mass. In combustion processes, these characteristics affect heat and mass transfer, critical factors in the design of efficient combustion systems. Kinetic isotope effects are used not only for fundamental studies but also for the validation of advanced numerical models that simulate the behavior of fuel mixtures [17]. Deuterium, through heavy water, ensures the efficient operation of nuclear reactors without requiring fuel enrichment. At the same time, tritium is considered the key to the development of future fusion reactors, such as ITER and DEMO, due to its favorable characteristics in D–T reactions [14]. In the current context of decarbonization and the transition towards a climate-neutral economy, the isotopes of hydrogen play an essential role through the diversity of their applications. Protium remains the main energy vector used in combustion processes and fuel cells, contributing to the reduction of CO_2 emissions. Deuterium and tritium, on the other hand, support the development of advanced nuclear technologies, providing long-term solutions for the production of clean and sustainable energy. The integration of this knowledge into current energy projects is essential for achieving climate neutrality objectives and ensuring a sustainable energy future.

1.4. Obtaining Technologies of Hydrogen Isotopes

This chapter presents the main technologies for obtaining hydrogen isotopes, covering both established industrial processes and emerging ones. The methods of producing protium (^{1}H), widely used, deuterium (^{2}H), valuable in research and nuclear applications, as well as tritium (^{3}H), relevant for controlled fusion, are analyzed.

1.4.1. Hydrogen Production from Hydrocarbons

Natural gas, composed mainly of methane, currently represents the most accessible, efficient, and economical source for producing hydrogen on an industrial scale. This method contributes approximately 70% to global hydrogen production. The use of existing infrastructure for natural gas distribution constitutes a significant advantage, facilitating the large-scale implementation of this production process [18]. Hydrogen can be obtained by the conversion of hydrocarbons, especially natural gas, using three main chemical processes: (i) partial oxidation, (ii) steam methane reforming, and (iii) autothermal reforming.

1.4.1.1. Steam Methane Reforming

The most widely used method for obtaining hydrogen is steam methane reforming (SMR), which is a mature and technically efficient technology, but associated with significant carbon dioxide emissions, estimated between 9 and 12 tons for each ton of hydrogen produced. The method involves high energy consumption, determined by the need to generate large amounts of superheated steam, both to maintain a H_2O/CH_4 molar ratio close to 3, and to reach the operational temperatures required in the active zone of the reactor [27]. The main chemical reaction is endothermic, requiring a continuous supply of thermal energy, and can be described as follows:

$$CH_4 + H_2O\left(+\frac{21MJ}{kmol\ CH_4}\right) \rightarrow CO + 3H_2 \quad (1)$$

The main product is a mixture of hydrogen and carbon monoxide, and in order to increase the hydrogen yield, a subsequent stage takes place called the water-gas shift reaction. In this reaction, carbon monoxide reacts further with steam, forming carbon dioxide and hydrogen:

$$CO + H_2O \rightarrow CO_2 + H_2 + \frac{41MJ}{kmol\ CO} \quad (2)$$

In order to reduce the environmental impact, carbon capture and storage (CCS) technologies are being developed and implemented. CCS can capture up to 90% of CO_2 emissions, but it involves significant investments in infrastructure [28]. A complementary alternative consists in replacing the conventional thermal source with energy supplied by nuclear reactors, thus eliminating the dependence on fossil fuels in generating the steam required for the reforming process.

1.4.1.2. Partial Oxidation Reforming

In addition to the optimization of the SMR process, another widely applicable industrial method for obtaining hydrogen is the partial reforming of methane (partial oxidation). Partial oxidation is an exothermic process, characterized by heat release. Compared to steam reforming, the reaction takes place in a significantly shorter time and requires a smaller reactor volume. However, the hydrogen conversion yield is lower, since the amount of hydrogen obtained per unit of fuel introduced is inferior to that of steam reforming.

1.4.1.3. Autothermal Reforming

A hybrid method, which combines the advantages of steam reforming and partial oxidation, is the autothermal reforming of methane (ATR). This technology simultaneously uses steam and oxygen in the feed mixture, allowing the balancing of energy input and consumption within the same process.In ATR, the thermal input required for the endothermic reactions is provided through the partial oxidation of methane, both reactions taking place within a single reaction volume. The main objective of ATR is to obtain a synthesis gas with a high hydrogen content, under the constraints imposed by thermodynamic equilibrium. However, the constraints imposed by the need to reduce the carbon footprint require the re-evaluation of these technologies in the context of decarbonization objectives. In this regard, the integration of solutions such as carbon capture and storage (CCS), the use of renewable heat sources, or the transition towards non-polluting methods, such as water electrolysis with renewable energy, becomes essential for the future of sustainable hydrogen production.

1.4.2. Hydrogen Production through Water Electrolysis

Another raw material used for obtaining hydrogen, which allows the integration of renewable energy sources, is water. Electrolysis consists in applying an electric current through an electrolytic solution or a solid medium to separate water into its elemental components. Since it does not involve direct greenhouse gas emissions, this method is considered climate-neutral and sustainable [46]. If the electricity used comes from renewable sources (wind, solar, hydro) or from nuclear sources, electrolysis becomes a zero-emission hydrogen production technology.

1.4.3. Emerging Energy Source – Natural Hydrogen

Natural hydrogen, a form of molecular hydrogen that forms and accumulates naturally in the Earth's crust, has recently become a new direction of interest in the field. Currently, estimates indicate that approximately 20 Mt/year of natural hydrogen escapes into the atmosphere [49], much of it reaching the ionosphere and being lost into space [50]. Its formation is attributed mainly to the geochemical process of serpentinization. Although it was previously believed that exploitable accumulations of natural hydrogen could not exist, recent studies have identified geological formations in which hydrogen is continuously released [51]. Overall, natural hydrogen has the potential to support the decarbonization of several industrial sectors – refineries, methanol production, ammonia – as well as the transportation sector, through new e-fuels or the use of ammonia. Local hydrogen-based energy production is a viable alternative, and the blending of hydrogen with natural gas for heating (already implemented in the United Kingdom) confirms compatibility with existing infrastructure [85, 86]. For industrial processes requiring high temperatures (e.g., steam cracking, cement kilns), hydrogen is a promising alternative to fossil fuels [87]. The integration of natural hydrogen into the economy can accelerate the transition towards a sustainable, low-carbon future. An innovative direction in hydrogen production is represented by the conversion of plastic waste into hydrogen. According to a recent study published in Nature Catalysis, this method allows the extraction of more than 97% of the hydrogen mass contained in plastics, using a simplified technological process. This approach promises not only an alternative source of hydrogen but also a sustainable solution for the recovery of plastic waste, simultaneously contributing to the reduction of microplastic pollution and the decarbonization of industrial processes [58].

1.4.4. Methods for Obtaining Deuterium and Tritium

ICSI Râmnicu Vâlcea has developed and validated at laboratory scale a combined technology for the separation of D and T from deuterated/tritiated water (catalytic isotopic exchange + cryogenic distillation), transferred into a semi-industrial pilot installation equivalent to a detritiation unit for CANDU-type heavy water, with the direct purpose of application at Cernavodă NPP. The research targets scalable technologies, with optimized energy consumption and high isotopic selectivity, essential conditions for the industrial feasibility of hydrogen isotope separation [59]. Although there are more than one hundred methods for deuterium separation, the industrial production of heavy water is based on isotopic exchange and distillation, while other techniques remain predominantly analytical; classical methods (cryogenic distillation, thermal diffusion, chromatography) are limited by complexity and energy costs [16, 60]. In modern practice, processes such as CECE and LPCE/VPCE often integrated with cryogenic distillation — are central both in ICSI solutions and in the detritiation systems at ITER [61]. Cryogenic distillation of hydrogen remains the reference for obtaining high-purity D/T, supported by mathematical models for multicomponent columns (Lewis-Matheson, Underwood, dynamic simulations) [61, 62, 63, 64], while membrane approaches indicate promising separation factors (up to 5.66) for deuterium-lean mixtures [65–67]. In this context, the CTRF project at Cernavodă NPP advances the implementation of cryogenic and catalytic solutions for the reduction of tritium in heavy water, consolidating the role of ICSI as a center of excellence and facilitating the transfer to emerging energy applications [69].

1.5. Challenges, Safety, and Future Perspectives

The use of hydrogen isotopes, especially deuterium and tritium, brings important technological benefits in industrial and nuclear processes, but also involves technical, safety, and regulatory challenges. The main difficulties concern the efficiency of isotopic separation, high energy consumption, and the complexity of installations, particularly in the case of tritium technologies such as cryogenic distillation and catalytic exchange. Additional problems arise from permeation and material corrosion, catalyst degradation, and the need for robust solutions for continuous operation. In nuclear fusion, the integration of the D–T fuel cycle requires efficient tritium recovery and recycling, managed under strict safety conditions, given its radioactivity and contamination risks. The lack of complete international standards complicates transport and handling, which emphasizes the need for clear regulations. Recent advances in advanced materials, mathematical models and predictive simulations, along with emerging technologies such as artificial intelligence and miniaturized sensing, provide promising perspectives for process optimization and reduction of environmental impact. In this context, the reuse and recovery of isotopes become essential components for a circular hydrogen economy, with a strategic role in the global energy transition.

1.6. Hydrogen Purity: Key Factor in the Choice of Production Technology

The purity of hydrogen is essential for advanced applications such as fuel cells, the semiconductor industry, and precision chemical processes, requiring levels between 99.5% and over 99.9999%. The choice of purification method depends on the composition of the raw gas, the type of impurities, and the purity requirements, and the technologies used include mechanical processes (PSA, VSA, TSA, membranes, cryogenic distillation), chemical processes (metal hydrides, catalytic purification), and physical processes (mass-based or diffusion separations) [70–72]. Pressure swing adsorption (PSA) is the dominant industrial method, but recent research explores hybrid solutions with membranes and cryogenics, capable of significantly reducing energy consumption and increasing recovery rates [80–82]. Palladium-based metallic membranes can ensure ultra-high purity (99.999%) [86], while cryogenic distillation remains the standard for obtaining very high purity H_2, though with high energy costs [89]. The integration of hybrid methods and advanced contaminant control provides promising solutions for the sustainable production of hydrogen, facilitating the transition towards the hydrogen economy [91].

1.7. Applications of Hydrogen Isotopes in Industry and Energy

Hydrogen is a versatile energy carrier, with major industrial and energy applications, from the production of ammonia and methanol to hydrocracking, desulfurization, and the direct reduction of iron ores, playing an essential role in the transition towards a low-carbon economy [92, 93]. In the energy sector, it is used for renewable energy storage, fuel cell supply, integration into gas networks, and the production of synthetic fuels. In this context, its isotopes have specific uses: deuterium (D_2O) as a moderator in nuclear reactors and as a solvent/tracer in pharmaceutical and spectroscopic applications, and tritium, a radioactive isotope, in nuclear fusion, luminescent sources, medical applications, and environmental research [46]. The unique characteristics of deuterium and tritium make them strategic fuels for nuclear fusion, considered a clean and sustainable source of energy, and isotopic separation becomes essential for supplying research and cutting-edge technologies in the energy field and materials science [46].

Chapter 2: Green Hydrogen – Energy Vector

The hydrogen-based economy represents one of the fundamental directions of the energy transition, aiming at the gradual renunciation of fossil fuels. At present, hydrogen production is largely based on natural gas, considered a promising substitute for coal and oil due to its relatively reduced greenhouse gas emissions [94]. Climate neutrality scenarios include the massive increase in renewable energy production (photovoltaic, wind, bioenergy), the application of carbon capture and storage/utilization technologies (CCS/CCU), the development of synthetic fuels (CH_4, CH_3OH, NH_3), and the integration of green hydrogen as a multifunctional energy vector, used for storage, transport, and grid balancing. In this equation, Power-to-X (PtX) technology, and especially Power-to-Gas (PtG), plays a central role by converting renewable energy into hydrogen and gaseous fuels, with extended storage possibilities and applications in transport, industry, and households. Water electrolysis constitutes the core of PtX processes. Alkaline electrolyzers (AEC) are the most mature and widespread, characterized by robustness, reliability, and lower costs compared to emerging technologies. They use a KOH-based alkaline solution and achieve efficiencies of 66–74%, corresponding to a consumption of approximately 51 kWh/kg H_2. The lifetime of modern systems exceeds 60,000 hours, and current investment costs in Europe are around ~500 EUR/kW. The levelized cost of hydrogen (LCOH) obtained ranges between 2.5–3.7 USD/kg H_2, with estimates for 2030 indicating drops below 2.0 EUR/kg due to technological progress and economies of scale [95–97]. Proton exchange membrane (PEM) technology offers superior operational flexibility, with reduced start/stop times, rapid response to load variations, and efficient operation in transient mode, which makes it ideal for integration with variable renewable sources. Its limitations are related to high costs (CAPEX), the use of noble metal-based catalysts, and membrane degradation, but significant reductions are anticipated through design optimization and increased industrial production [98–100]. A promising research direction is represented by solid oxide electrolyzers (SOEC), which operate at high temperatures (700–850 °C) using ceramic electrolytes. These can achieve efficiencies of 75–80% through the integration of external thermal energy, reducing electricity consumption. Exergy analyses have shown an increase of up to 11% in exergy efficiency compared to low-temperature technologies, but high costs and reduced maturity currently limit industrial implementation [101]. At the European level, the costs of green hydrogen currently vary between 3.3–3.7 EUR/kg H_2 in Romania [101], 5–8 EUR/kg H_2 in Central Europe [102], and about 5.6 USD/kg H_2 at the European Union level [103]. Projections for 2050 set a realistic horizon for technological and economic maturity, with large-scale implementation of electrolyzers and the development of Power-to-Gas infrastructure. In this context, pilot projects have been developed, such as WOMBAT (Germany), monitored through the dedicated European platform [104], or e-gas plants that transform surplus renewable energy into synthetic methane, confirming the feasibility of the technologies [105]. Other initiatives include the Romanian project 20HyGrid and the Spanish program Green Hysland, which demonstrate the integration of hydrogen into natural gas distribution networks.

From the perspective of storage and use, green hydrogen can be injected into methane (CH_4) networks, used in transport through fuel cells, in industry (ammonia, methanol), or in CO_2 methanation processes, generating synthetic fuels with a reduced carbon footprint. The design of burners dedicated to the combustion of H_2–CH_4 mixtures and the development of predictive models allow the optimization of combustion parameters and the reduction of pollutant emissions, essential aspects for industrial applicability. In this sense, experimental and numerical research dedicated to the combustion of H_2–CH_4 mixtures can contribute to the development of innovative solutions for the transition to a sustainable hydrogen-based economy.

Chapter 3: Technological Particularities of the Combustion of Gaseous Fuel Mixtures, including Hydrogen–Methane for the Energy Transition

3.1. *Hydrogen and the Energy Transition: Challenges and Opportunities*

The goal of the energy transition is the reduction of greenhouse gas emissions, and hydrogen is becoming an essential energy vector due to its carbon-free use. An intermediate solution is represented by hydrogen and methane mixtures (H_2–CH_4), which can be transported through existing gas networks, allowing a gradual transition without major investments. At the current stage, it is recommended to limit hydrogen to 15%, with perspectives of increasing to 30% in the medium term. However, implementation involves technical, economic, and regulatory challenges, but it also offers opportunities for reducing dependence on fossil fuels. In this context, combustion technologies and the development of burners adapted for H_2 or H_2–CH_4 mixtures play a crucial role in harnessing the potential of hydrogen in the energy transition.

3.2. Characteristics of Gaseous Fuels

Any gaseous fuel consists of a mixture of combustible gases, inert gases, and water vapor. Gaseous fuels are either natural or artificial. Natural gas consists mainly of methane. It can be obtained from its own deposits, non-associated with crude oil, or from gas associated with crude oil, obtained at the same time as it.

3.2.1. Volumetric Composition

The volumetric composition includes the participation of each component of the gaseous fuel, expressed in volume percentages. It is expressed in the anhydrous state or in the wet state (also called initial). The two states result from the condensation of water vapor when determining the volumetric composition. The humidity of the fuel is noted with d and is expressed in grams for one m_N^3 of dry gaseous fuel.

3.2.2. Quality of Gaseous Fuels

Natural gases associated with oil fields exploited on the territory of Romania, obtained as by-products in the oil extraction process, are composed predominantly of light hydrocarbons (methane, ethane, propane, and butanes), along with variable fractions of inert gases or impurities (such as carbon dioxide). Knowing their composition is essential both for assessing the energy potential and for determining pretreatment measures and efficient industrial use. The data show a high similarity between the two types of gas, especially due to the dominant proportion of methane (which can exceed 97–98% in certain deposits), which gives the natural gas from Transylvania remarkable purity. This high purity often justifies the use of the expression that natural gas from the region can be confused with pure methane in terms of thermodynamic behavior, energy value, and combustion characteristics. This compositional and energetic similarity has important technical implications: it allows the direct use of natural gas in high-performance industrial applications without the need for complex pretreatment, ensures complete combustion with reduced emissions, and facilitates integration into transport and distribution networks designed for methane. In addition, the similarity with pure methane contributes to the standardization of the design and operation processes of thermal and energy equipment. It is noteworthy that hydrocarbons (such as methane, ethane, propane, or butane) have high calorific values, increasing with molecular mass. Hydrogen, although it has the lowest density, offers significant energy content relative to its own mass. Gases such as nitrogen, oxygen, or carbon dioxide have no calorific value but can influence the combustion process when present in mixtures. This information is useful in the selection of gaseous fuels depending on the desired application and energy efficiency requirements.

3.2.3. Fuel Mixtures

Special attention is given to the calorific value and caloric participation in the context of the simultaneous use of two or more gaseous fuels. If the calorific value of one gas in the mixture is noted as $H_i^{i_1}$ and that of the other as $H_i^{i_2}$, with the volumetric participation of the first gas in the mixture being r_1, the calorific value of the mixture is determined with the following relation:

$$H_{i,am}^{i} = r_1 * H_i^{i_1} + (1 - r_1) * H_i^{i_2}, [kJ/(m_N^3)] \quad (3.12)$$

The heat (thermal) participation in percentages, q_1, of the first gas in the mixture will be:

$$q_1 = \frac{100 * r_1 * H_i^{i_1}}{r_1 * H_i^{i_1} + (1 - r_1) * H_i^{i_2}}, [\%] \quad (3.13)$$

The calorific value of a mixture of gaseous fuel with a liquid fuel is determined using the following relation:

$$H_{i,am}^{i} = H_i^{i_1} + n * H_i^{i_2}, [\text{kJ/kg}] \quad (3.14)$$

where $H_i^{i_1}$, [kJ/kg] is the calorific value of the liquid fuel, and $H_i^{i_2}$ is the calorific value of the gaseous fuel, $[kJ/(m_N^3)]$. n denotes the ratio between the flow rate of the gaseous fuel and that of the liquid fuel, $[m_N^3/kg]$. The caloric participation q_2 of the gaseous fuel in the mixture with the liquid fuel is determined using the relation:

$$q_2 = \frac{100*n*H_i^{i_2}}{Q_i^{i_1}+n*H_i^{i_2}}, [\%] \quad (3.15)$$

3.2.4. Physicochemical Properties of H_2–CH_4 Mixtures

Hydrogen and methane mixtures exhibit physicochemical characteristics distinct from conventional natural gases, influencing the way they can be used. The combustion process of hydrogen takes place without producing carbon dioxide, particles, or other pollutants, except for nitrogen oxides (NOx) [107]. It can be observed that from a volumetric point of view, hydrogen requires less air than methane for stoichiometric combustion, but from a mass point of view, the opposite is true. In terms of calorific value, hydrogen stores a much larger amount of energy per kilogram than methane, whereas volumetrically the opposite applies. Since the molecular mass of methane is approximately eight times higher than that of hydrogen, the combustion of one methane molecule releases about three times more heat than the combustion of one hydrogen molecule. Hydrogen has a higher auto-ignition temperature and higher thermal conductivity than methane [108]. Due to the differences in the laminar burning velocity values of the two gases, design modifications will be necessary for burners. Since hydrogen is more soluble in materials, its leakage rates in distribution systems are higher than those of methane gas, an aspect important both from a safety and economic point of view. For safe and efficient operation, hydrogen burners require appropriate design and operation. However, additional safety measures are necessary, given that hydrogen is extremely flammable. Hydrogen ignites easily in the atmosphere, with a flammability range between 4.65% and 93.9% in oxygen, while in air this range varies between 4% and 75% [109]. The combustion of pure hydrogen presents risks due to its wide flammability range and the low energy required to initiate the combustion reaction, generating safety concerns. siguranță.

3.3. Elements of Combustion Theory for Gaseous Fuels

3.3.1. Physical and Chemical Processes

It has been found that the flame propagation mechanism of gaseous fuels also includes reactions with alkyl radicals, OH, and free oxygen and hydrogen atoms. For the physical part of combustion, the so-called thermogasodynamic transfer parameters must be known: thermal conductivity, molecular diffusion coefficient, and thermal diffusion coefficient. An analogy can be made between heat transfer by convection (characterized by the Nu criterion) and mass transfer (characterized by the Nu_dcriterion). Generally, simultaneously with the molecular diffusion process, there is also a displacement of substance through convection, the convective flux being equal to the product between the velocity u of the stream and the mass concentration C.

3.3.2. Elements of the Combustion Theory of Gaseous Fuels

From the point of view of the physical process, the combustion of gaseous fuel includes two technologies. Thus, kinetic combustion is distinguished, when there is a premix of fuel and oxidant, and diffusive combustion, when the contact of the fuel with the air takes place in the flame zone.

3.3.2.1. Kinetic Combustion of Gaseous Fuels

A mass element of gaseous fuel–air mixture first receives heat through conductivity. As a result, the temperature increases from the initial value T_0 to the value T_1, when the volume element begins to release heat. The chemical reactions will lead to the increase of the temperature from the value T_1 to the value T_f. The normal burning velocity is perpendicular to the flame front and opposite in direction to the flow direction. Depending on the flow regime, the normal burning velocity is distinguished for laminar flow, SL, and respectively for turbulent flow, ST. The normal burning velocity in turbulent flow regime is higher than that for the laminar flow regime. There are several models to define the burning velocity in turbulent flow regime. The Damköhler model is based on the deformation of the flame front under the action of turbulence. The Karlovitz model considers the development of the turbulent flame as a result of laminar flow combined with turbulent diffusion. The processing of experimentally obtained data led to a new concept, namely turbulence generated by flame development. The Summerfield model considers the turbulent flame as a zone of dispersed reactions, propagated on the basis of laminar flame theory. The excess air in the fuel–air mixture is called the degree of aeration. The decrease of flame stability occurs with the increase of the degree of aeration. Thus, for fuels with low molar mass or with hydrogen molecules, stability is maximum for stoichiometric concentrations or with a slight shift towards the lean mixture. On the contrary, for heavy hydrocarbons, the stabilization domain is towards the fuel-rich mixture. The stability limits increase with increasing temperature.

3.3.2.2. Vortical Flow (Swirling Jets)

Stability through the rotation of jets (swirling of jets) is a generally valid method for all types of flames and for any fuel. Flame stability is due to the internal recirculation that occurs in the low-pressure central zone of the swirling jet. Swirling jets, also called rotational jets, are generated by special devices placed in the body of the burner. The characteristic of a swirling flow consists in the existence of a spatial velocity vector, in which the axial and tangential components dominate. Depending on the magnitude of the rotational character of the flow, in the central zone there also appears a recirculation current with reverse axial flow.

3.4. Diffusive Combustion of Gaseous Fuels

The process is characterized by the mixing of air and gaseous fuel outside the burner body. The flame shape depends on the excess of air. When the flow velocity of the fuel increases, the flame length increases progressively, but once the turbulent flow regime is reached, the flame length stabilizes, and the flame becomes noisy. For the diffusive flame, it can be assumed that it is very stable, since flame blow-off can only occur when the velocity on the jet axis in the section where the stoichiometric concentration is achieved exceeds the burning velocity for that point ($u_m \leq S_T$).

3.4.1. Free Jets

The burning velocity in turbulent flow regime, S_T, has a profile that results from the minimum value for high fuel concentrations (in the central zone) and for low fuel concentrations (at the jet periphery), and from the maximum value in the stoichiometric fuel–air concentration zone. In a simplified way, a free fuel jet is considered. The development velocity of the combustion process in diffusive regime is determined only by the diffusion velocity between the gas and the air. The diffusion process takes place in the direction perpendicular to the flow direction.

3.4.2. Fuel Jets Accompanied by a Constant Velocity Air Stream

The fuel jet is accompanied by an infinite parallel air stream with velocity u_{o2}. If the ambient velocity is zero ($u_{o2} = 0$), the upper blow-off velocity ($(u_{or})^s$) becomes equal to u_{or}, and the lower blow-off velocity becomes zero, $(u_{or})^i = 0$. As the velocity of the accompanying stream u_{o2} increases, the value of the lower blow-off velocity decreases (resulting in a decrease of the flame stability domain).

3.4.3. Fuel Jets Accompanied by Variable Ambient Velocity

For this situation, for the velocity field at various sections of the jet, the integral momentum conservation equation is used. Here, I_1 and I_2 represent the initial momentum of the central jet and, respectively, of the peripheral jet. Tf is the flame temperature; σ is the ratio between the number of moles entering the reaction and the number of moles resulting from the reaction; T_0 is the initial temperature at the exit from the burner port.

3.4.4. Confined Jets

Compared to a free jet, a confined jet has as its main characteristic the interaction with the combustion chamber (furnace). As a result, there must be a close correlation between the development of the jet and the dimensions of the combustion chamber. The momentum of the jet is transformed for the most part into static pressure. The amount of fluid surrounding the jet is limited, so if m_0 is the mass of fluid exiting the burner and m_a the mass of fluid entrained from the surrounding medium, the fluid concentration at the end of the combustion chamber will be $C_\infty = m_0/(m_0 + m_a)$. It follows that confined jets are not self-similar like free jets, but depend on the recirculation parameter. At the moment when the jet intersects the walls of the combustion chamber, the concentration C_∞ is reached.

3.5. Types of Burners for the Use of Hydrogen

In the context of using hydrogen–methane mixtures in natural gas networks, one of the significant challenges is the adaptation of combustion equipment, including burners. Burners must therefore be designed to respond to the particularities of hydrogen, such as its very high burning velocity with the formation of stable flames, which requires innovative technical solutions.

3.5.1. Premix Burners

Premix burners are used both in residential heating boilers, where they ensure efficient combustion and reduced pollutant emissions, and in cooking appliances, such as stoves. A gas boiler represents a system used to produce heat through the combustion of a premix of natural gas or hydrogen–methane mixtures with air. The burner ensures the optimal mixture between fuel and air, guaranteeing efficient combustion and the reduction of pollutant emissions. The gas supply is controlled through a gas valve, which regulates the fuel flow rate and contributes to optimizing combustion. For safety, the system is equipped with a shut-off valve, which automatically interrupts the gas supply in case of malfunctions or leaks. The heat exchanger facilitates the transfer of thermal energy from the combustion gases to the heating agent, optimizing the energy efficiency of the system. The combustion gases resulting from the process are evacuated outside through an exhaust vent, in compliance with safety regulations

and environmental protection. The operation of the boiler is controlled through the thermostat and the control panel, which monitor and adjust parameters for maximum efficiency. By integrating these components, the heating boiler operates efficiently, offering a safe and economical heating system for various residential and industrial applications. Combustion process control is used only for burners that utilize premixed mixtures. When using up to 20% hydrogen in the methane gas flow, no flashback observations were found for this type of burners. In the context of describing the classic premix burner, it is important to mention that current research continues to explore and improve the performance of this type of equipment. Article [118] describes a study that includes both experimental and numerical analyses carried out on a premix burner derived from an industrial unit that uses natural gas. The purpose of the design of this type of burner was to reduce the distance between the premixer and the actual gas turbine burner, in order to optimize the combustion process and the performance of the system. The burner was tested using methane gas, hydrogen–methane mixtures, and even pure hydrogen, in a combustion testing facility that simulates combustion conditions at atmospheric pressure. The results showed that during hydrogen operation, the exit velocity of the gases resulting from the combustion process (80 m/s and 130 m/s) is higher than when the burner operates with natural gas. In addition, nitrogen oxide (NOx) emissions were measured and flame flashback limits were determined for the two burner configurations. To enable a gradual transition for medium and high thermal power from burners using methane gas to hydrogen use, operation was carried out with diffusive combustion technology. This approach allows the adaptation of existing equipment to use hydrogen before making the complete transition. In the scientific analysis [121], it is highlighted that the combustion of hydrogen–methane mixtures is part of the practical short- and medium-term strategy for achieving decarbonization. A hydrogen/methane mixture with 20% hydrogen by volume leads to a reduction of CO_2 emissions of approximately 7%. Increasing the hydrogen content to 30% leads to a reduction of slightly more than 10%.

3.5.3. Self-Aspirating or Atmospheric Burners

These burners are applied in low-flow thermal installations (hot water and steam boilers and some industrial furnaces). The air is aspirated directly from the atmosphere (it is not preheated). Self-aspirating burners generally operate with low-pressure natural gas. As a result of mixing the fuel with air in the diffuser, a flame with kinetic combustion is obtained. To increase combustion stability, it becomes almost mandatory to equip with a flame stabilizer at the burner outlet section.

3.6. Conclusions

This work has addressed in an integrated manner the issue of using hydrogen as an energy vector in the context of the energy transition, with emphasis on the particularities of combustion processes and the technological solutions adapted to this fuel. The analysis carried out highlighted that the adoption of hydrogen in the energy mix requires a profound reassessment of the physicochemical characteristics of gaseous fuels, of combustion phenomenology, and of the constructive configurations of combustion equipment. Regarding the characteristics of gaseous fuels, significant variations in their composition and quality were identified, with direct implications on combustion processes, flame stability, thermal efficiency, and pollutant emissions. The behavior of H_2–CH_4 mixtures reveals a series of particularities, among which stand out the high flame propagation velocity and the increased potential for nitrogen oxide (NOx) formation, imposing additional requirements for combustion control and optimization. The chapters dedicated to combustion theory provided a rigorous framework on the physicochemical mechanisms involved, as well as the behavior of turbulent jets under various flow and mixing regimes. In particular, the diffusive combustion of gaseous fuels was analyzed from the perspective of the interaction between fuel jets and air streams, also considering the relevant criteria characterizing the recirculation process and mixture efficiency. Regarding burner technology, various configurations compatible with hydrogen use were examined: premix burners, diffusive flame burners, self-aspirating burners, and low-NOx burners. It has been demonstrated that the efficiency of these solutions is conditioned both by the internal architecture of the combustion system and by the possibility of precise control of operating parameters, especially the air–fuel ratio and tertiary air distribution. NOx emission control remains a priority objective, achievable through advanced mixing techniques, exhaust gas recirculation, and optimized burner architectures. Research perspectives include the development of hybrid solutions, real-time control algorithms, and experimental validations for real operating conditions.

Chapter 4: CFD Simulation of a Diffusive Burner for Methane and Hydrogen Mixtures: Performance and Challenges

The research carried out investigates through numerical simulation the operation of a diffusive burner designed for the combustion of hydrogen and methane mixtures, with a hydrogen concentration of up to 50% in methane. To solve the problem, advanced computational fluid dynamics (CFD) methods were used within the ANSYS Fluent platform. The main objective of the research is the overall analysis of combustion processes – flame stability, temperature distribution, and the level of gaseous emissions – in the context of promoting the use of alternative fuels with low carbon emissions. The developed model reproduces a diffusive burner operating within industrial limits, under controlled flow rate and fuel mixture composition conditions. The results obtained highlight the optimal operating conditions of the burner and underline the potential of hydrogen and methane mixtures as a transition solution towards a hydrogen-based economy. The study provides relevant information for the design and operation of burners compatible with alternative fuels. Through these contributions, the research supports a better understanding of the combustion mechanisms specific to diffusive burners and proposes technological solutions aimed at reducing the environmental impact in the energy sector.

4.1. Introduction

The diffusive combustion of the gaseous H_2–CH_4 mixture has included multiple studies based on numerical modeling. This approach includes the advantage of realizing the interaction between turbulence and chemical reactions. These aspects determined through numerical modeling formed the basis for the constructive design and sizing of burners. Of particular importance is the definition of chemical species and the chemical reactions in which they are involved [122]. The most commonly encountered viscosity model is WALE (Wall Adapting Local Eddy Viscosity). The aim is: recovering viscosity to real values near the walls and preserving dispersion properties for damping turbulence in the transition from laminar to turbulent flow. The probability density function (PDF) method was used as an SGS closure solution in LES. The conclusions drawn from numerical modeling studies of H_2–CH_4 gas combustion are: ignition and burning of the H_2 component in the first part of the generated flame; the maximum values of CO mass fraction are in the center of the flame, with the highest concentration in its first third; the H_2 component proportionally increases the axial velocity of the flame; combustion excess is essential for NOx emission. Hydrogen is considered a fuel with high future use potential, against the background of fossil fuel resource depletion and increasing air pollution levels. In particular, the continuously increasing concentration of carbon dioxide in the atmosphere stimulates the transition to more sustainable energy solutions. Hydrogen stands out through a series of significant advantages, such as clean and efficient combustion, high refueling speed, high energy storage density, and its availability as a renewable resource. In addition, hydrogen combustion does not produce greenhouse gases such as carbon dioxide, but only water vapor, which makes it an essential ally in reducing carbon emissions and combating climate change. The expansion of hydrogen use as an energy vector presents considerable potential in reducing pollutant emissions and, implicitly, in improving air quality, with direct positive effects on the environment and human health. Due to its favorable characteristics – such as the absence of carbon dioxide emissions during combustion and the possibility of being produced from renewable sources – hydrogen emerges as a viable long-term energy solution, capable of responding to increasingly stringent requirements regarding sustainability and energy security in the context of the transition to a decarbonized energy system. The hydrogen combustion process takes place without generating carbon dioxide emissions, particles, or other pollutants, except for nitrogen oxides (NOx) [133]. Thus, hydrogen is considered a zero-emission energy vector, since it does not contribute to atmospheric pollution. It can replace fossil fuels in a variety of applications, including in industry and the residential sector, contributing significantly to reducing environmental impact [134]. Compared to natural gas, hydrogen presents significant differences in terms of physicochemical characteristics, such as calorific value, flow and combustion properties, thermal characteristics, density, flame propagation velocity, and interaction with the distribution network. The blending of hydrogen in small amounts, up to 15% in the natural gas flow, induces moderate changes in its characteristics; however, these changes are acceptable in the context of the objective of decarbonizing gas networks. According to the specialized literature, the addition of even up to 30% hydrogen in methane can be industrially implemented and managed safely, without significant risks. [135 – 136]

4.2. Burner Configuration/Geometry

The burner consists of two distinct chambers, each chamber being equipped with nozzles dedicated to fuel supply and, respectively, air. The fuel is introduced into the combustion zone through five pipes (nozzles) with an inner diameter of 4 mm, symmetrically arranged to ensure a uniform distribution of the flow. The combustion air is

supplied from the air chamber and enters the flame through an annular space arranged around each fuel nozzle, thus ensuring a controlled and balanced supply of oxidant in the reaction zone. To optimize the mixing process and avoid the formation of composition inhomogeneities, each chamber is equipped with a perforated plate, whose role is to homogenize the flow of both fuel and air before entering the actual combustion system. The arrangement and geometry of the perforations are rigorously designed so as to reduce the formation of turbulent jets or stagnant zones, factors that can compromise the uniformity of flow distribution and the stability of the flow regime. Moreover, non-uniform combustion can favor a spatial imbalance of the flame in the formation of soot deposits. In particular, for hydrogen and methane mixtures, the control of mixture distribution becomes even more critical due to the specific properties of hydrogen, such as its much higher flame propagation velocity and extended flammability range.

4.3. Non-Premixed Combustion Modeling Using the k–ε Turbulence Model in ANSYS Fluent

In the research carried out, the combustion process was simulated using ANSYS Fluent, by implementing the non-premixed combustion model in combination with the standard k–ε turbulence model. This approach allowed for robust prediction of the temperature field, the distribution of chemical species, and the formation of pollutant emissions, providing a detailed understanding of the thermochemical phenomena associated with the combustion of hydrogen and methane mixtures in the flame.

4.3.1 Geometric Modeling and Domain Discretization

The physical model of the burner was created through three-dimensional modeling of the burner at scale, using CATIA V5 software. The resulting geometry was later imported into ANSYS Fluent, where the flow volumes corresponding to the fuel and air were defined. Discretization was carried out using an advanced mesh generation algorithm, optimized to balance the number of elements with their geometric quality. This approach enabled the development of a coherent mesh, with a reasonable computational cost, ensuring adequate resolution for capturing turbulent phenomena in the combustion zone.

4.3.2. Numerical Settings in ANSYS Fluent

The simulations were performed using the following options and configurations:

- Pressure-based solver, suitable for incompressible or weakly compressible flows [134];
- Steady-state simulation, appropriate for capturing the stationary behavior of the flame;
- State Relation: Chemical Equilibrium, assuming instantaneous equilibrium between the chemical species involved [138];
- Non-adiabatic energy treatment, allowing heat exchange between the combustion fluid and the domain walls.

4.3.3. Boundary Conditions

Input Conditions

At the domain inlet, the following boundary conditions were imposed: Velocity Inlet profiles for fuel and air; fuel concentration; turbulence intensity of 5%; turbulent/laminar viscosity ratio set to 10. These inlet conditions ensure a realistic development of the turbulent field and facilitate correct prediction of the fuel–oxidant mixture [133].

Wall Conditions

The domain walls were treated based on the following assumption: Non-adiabatic (allowing heat exchange), modeled using Standard Wall Functions for the treatment of the near-wall region [135]. This choice is justified in the case of developed turbulent flow regimes, as it reduces the requirements for fine discretization in the boundary layer, enabling more computationally efficient simulation.

Output Conditions

At the outlet, the following conditions were used: Pressure Outlet with a gauge pressure of 0 Pa, Backflow Pressure Specification set to Total Pressure. This approach ensures proper management of recirculation, if it occurs, and contributes to maintaining numerical stability at the outlet (an essential aspect in combustion simulations). [134]

4.3.4. Non-Premixed Combustion Model

The combustion model used is the non-premixed one, based on: Mixture Fraction (Z), Probability Density Function (PDF) [139]. The reactive properties of the system are evaluated through integration over the Probability Density Function (PDF), which allows a detailed description of the variability and randomness of chemical phenomena within the combustion process. In the simulation, the formation of nitrogen oxides (NO_x) was also taken into account, using the emission prediction models available in ANSYS Fluent, which allow accurate estimation of NO_x concentrations depending on combustion conditions and operating parameters [136].

4.3.5. Standard k−ε Turbulence Model

The modeling of the turbulent field was carried out using the standard k−ε model, which solves two additional equations for turbulent kinetic energy (k) and turbulent dissipation rate (ε). This model is widely used due to its simplicity and efficiency in simulating turbulent flows in many engineering applications [135]. The k−ε model is suitable for turbulent flow regimes with high Reynolds numbers and was chosen due to its robustness and numerical efficiency, being an effective tool in simulating turbulent flows in many engineering applications, including turbulent combustion cases [135].

4.4. Analysis and Interpretation of Numerical Simulation Results

4.4.1. Analysis of Flow Distribution Inside the Burner

The simulation process first included the analysis of the cold flow of fluids both inside the burner and at its outlet into the combustion space. Figure 4.3 shows the velocity profiles for the flow inside the burner, as well as in the area immediately adjacent to the inlet to the combustion chamber, for the fuel mixture composed of 50% hydrogen and 50% methane, with an excess air ratio $\lambda = 1$.

4.4.2. Analysis of the Combustion Process

The simulation matrix included 5 main cases: the variation of fuel composition and the air–fuel ratio expressed by the excess air λ. The simulation results were interpreted based on the evolution of flame temperature, the composition of the combustion gases (CO, CO_2, H_2O, NO_x), the turbulent kinetic energy, and the flame speed. Simulation 1, corresponding to the combustion of a mixture consisting of 100% CH_4, is considered the reference case for characterizing the combustion process, both in terms of the temperatures reached and the emissions generated. The main focus was on testing the combustion capacity with air drawn from the environment. However, high values of carbon monoxide (CO) emissions were observed, according to the dedicated graph. Simulation 2 is characterized by a real air–fuel ratio (AFR) of 17.6, corresponding to a lambda factor λ very close to the stoichiometric one, with additional air from the external environment, defined as the ratio between the real AFR and the stoichiometric AFR, equal to 0.9. Although $\lambda < 1$ indicates a decrease in the fraction of carbon monoxide (CO), this is also due to the presence of hydrogen. At the same time, the presence of H_2 contributed to the increase of the flame temperature and to the facilitation of ignition. Simulation 3 corresponds to a stoichiometric combustion regime, characterized by a lambda factor λ equal to 1. The increase in the air flow rate leads to greater efficiency of the combustion process, evidenced by the intensification of flame speed and turbulence, as well as by the reduction of carbon monoxide (CO) formation. In both Simulation 2 and Simulation 3, nitrogen oxides (NO_x) emissions remain at a relatively high level. Simulation 4 is characterized by a lambda factor (λ) of 1.3, corresponding to a combustion regime with excess air. The increase in air flow improved the combustion efficiency, as shown by both the intensification of flame speed and turbulence, and the reduction of carbon monoxide (CO) formation. The emission of nitrogen oxides (NO_x), compared to the previous simulations, was lower. Simulation 5 involved increasing the air flow up to a lambda (λ) value of 1.6. It can be observed that the maximum temperature reached is similar to that in the case with $\lambda = 1.3$, which suggests that additional excess air does not automatically lead to a significant reduction of flame temperature but contributes to improving the combustion process. This effect is supported both by the increased turbulence values and by the decrease in carbon monoxide (CO) concentration. The temperature peak is located much closer to the burner, which allows a more efficient heat transfer to possible heating surfaces. Analyzing the temperature evolution for the 5 simulation cases, a rapid increase in temperature is highlighted after leaving the burner, over a length of maximum 0.05 m. Only in one case, when the excess air is high, was a maximum temperature observed in an area farther from the burner, at about 0.17 m. The presence of hydrogen led to rapid ignition. The graphical representations obtained provide a detailed image of the thermal behavior of the flame and highlight the influence of fuel composition and excess air on the temperature distribution. In the case of pure methane combustion (100% CH_4, with an excess air coefficient $\lambda = 0.6$), a maximum flame temperature of approximately 1750°C was obtained, which remains relatively constant over a significant portion of the flame. By introducing hydrogen into the fuel mixture, a significant increase in reaction rate and an improvement in the homogeneity of the gas mixture are observed, due to the high diffusivity and reactivity of hydrogen. These characteristics led to obtaining higher maximum temperatures in the flame, as well as a more extended and uniform thermal distribution in the combustion space. The increase of excess air in the fuel mixture led to a significant modification of the flame structure. Thus, after reaching the core of maximum temperature—the area where chemical reactions are most intense and the energy release rate is maximal—a progressive decrease of the thermal value is observed along the flame axis. Research related to the influence of excess air values indicates an optimum in the range of 1–1.3. To explain this conclusion, new data from the

numerical simulation results were used, presented below. Through this approach, the three-dimensional behavior of the flame is highlighted, and it was possible to identify that there are no possible imbalances of supply or local turbulences that could affect thermal performance. Thus, a new confirmation results for the efficient solution of the pilot burner developed.

Evolution of combustion emissions (CO, CO_2, H_2O)

The evolution of the mass fractions of the combustion gas components was considered as a basis for a faithful representation of the combustion process. A rapid emission of H_2O indicates ignition and dominant combustion of the hydrogen component in the H_2–CH_4 mixture, as well as a delayed increase in CO_2 concentration. The delayed increase of the CO_2 component in the combustion gases indicates a flame in which hydrogen ignited and burned before methane. In the case of pure methane combustion (100% CH_4) at $\lambda = 0.6$, a high emission of carbon monoxide (CO) is observed, as a result of incomplete combustion due to lack of air, which indicates avoiding combustion with non-forced (atmospheric) air. Increasing the excess air does not change the previous conclusion regarding a flame initially represented by hydrogen combustion.

Evolution of NO_x emissions

Since NO_x formation is closely correlated with temperature and the duration of exposure to high temperatures, it was found that: for mixtures with 50% H_2 and stoichiometric combustion ($\lambda = 1$), NO_x emissions increase significantly due to the high maximum temperature; with the increase of excess air at values of $\lambda = 1.3$ and especially at $\lambda = 1.6$, NO_x emissions stabilize or decrease slightly, benefiting from the cooling effect generated by the excess air and the dilution represented by the excess air.

Analysis of turbulent kinetic energy

Turbulent kinetic energy represents an essential component in the analysis of turbulence phenomena in fluid flows, such as turbulent combustion. It measures the intensity of the pulsating motions of the particles in a fluid, having a significant impact on mixing processes, heat transfer, and chemical reactions. A maximum of turbulent energy was observed near the burner throat, resulting from the intense interaction between the fuel flow and the combustion air, accentuated by the rapid combustion reaction of hydrogen. Subsequently, the turbulent energy decreases rapidly after the ignition point. A second energy peak was recorded between 0.25 and 0.35 m, associated with the thermal expansion of the combustion products.

Evolution of flame speed

A significant increase in flame speed was observed with the increase in the hydrogen fraction and with air excess lambda (λ). To ensure flame stability, the injection velocity of the fuel and air at the burner nozzles must exceed the burning velocity, taking into account the complex decrease of velocity in the axial and radial directions. The recorded values of the flame flow velocity indicate that it exceeds the burning velocity in turbulent flow regime, thus demonstrating the complete stability of the simulated flames. The maximum burning velocity of hydrogen in laminar regime is approximately 3.1 m/s, while in turbulent regime the values vary in the range 1.0–3.0 m/s. Even for the methane combustion zone, corresponding to axial distances of 0.2–0.3 m, the flow velocity has values of over 3 m/s.

4.5. Conclusions

The numerical modeling highlighted high performance of diffusive combustion in hydrogen–methane mixtures with up to 50% H_2, using a real burner specially built for validation through experiments on a test stand. The simulations show flame stability in all studied cases; even at high velocities (case of excess air of 1.6) the flame remained attached to the burner orifices. The symmetrical distribution of temperatures and concentrations without major feeding imbalances or local turbulence confirms that the burner favors uniform mixing and good thermal control. By introducing hydrogen flow into methane, combustion is more complete with lower CO and CO_2 emissions, these being correlated with complete oxidation, while nitrogen oxide emissions can be controlled by adjusting the excess air..

Chapter 5: Experimental Research on the Combustion of $CH_4 - H_2$ Gas Mixtures

5.1. General Issues

The experimental research carried out aimed at validating the data obtained through modeling and numerical simulation. These led to remarkable results for the pilot burner designed and built for this purpose. The experimental test rig was designed and built in order to explore in detail the combustion process of hydrogen (H_2) and methane (CH_4) mixtures, incorporating the innovative burner presented in paragraph 5.2. Separate feeding with methane and hydrogen provides the flexibility to create variable mixtures of fuel gases. The design of the test rig was carried out so as to simulate real operating conditions. This makes it possible to obtain precise and valuable experimental data to support the development and optimization of experiments. In addition, the experimental rig is equipped with a wide range of advanced measuring and control instruments, which allow continuous monitoring of feeding and combustion parameters, such as flame temperature, pressure, and gas flow rate.

5.2. The Experimental Installation

General concept

The experimental installation included a specially designed and built test rig for the combustion of CH_4–H_2 mixtures in variable proportions. The rig also includes an original burner specially designed for the study of diffusive flames with applications for the following range of gaseous fuels represented by CH_4, CH_4–H_2, or even pure H_2. The separate feeding with methane and hydrogen imposed by the rig provides the flexibility to create variable mixtures of fuel gases, essential for a detailed study of flame behavior depending on the specific participation of the fuels used. The design of the rig was carried out so as to simulate real industrial operating conditions. The essential element of this experiment is the use of an innovative diffusive burner, which comprises 5 gaseous fuel jets each surrounded by the distribution of air through concentric jets. This concept allows a uniform flow distribution and dynamically controlled combustion, without significant fluctuations that could affect flame stability or process performance. In addition, the experimental rig is equipped with a wide range of advanced measuring and control instruments, which allow continuous monitoring of parameters such as pressure, gas flow, and flame temperature. The composition of the combustion gases was also monitored to ensure an optimized process, which would allow not only in-depth performance studies but also the evaluation of flame stability safety. In this sense, a process scheme was designed, the central element of which is the burner, pressure reducers connected to the gas sources, and flow control elements. The scheme allows feeding the burner with fuel and air under operational safety conditions. Thus, in addition to the gas control instruments used to obtain the desired methane and hydrogen proportions, check valves were also provided to prevent backflow and unwanted mixing, as well as a flame arrestor to prevent the formation and propagation of flame through the supply pipes.

The Diffusive Combustion Burner

The diffusive burner used in this experimental rig was designed to operate efficiently at atmospheric pressure, with an innovative design based on the use of concentric jets of fuel and air. This configuration ensures uniform and controlled combustion, in which the fuel mixture – a hydrogen and methane mixture – and the air are supplied through separate concentric channels. At the burner outlet, these gas and air streams mix, creating an optimal mixture for ignition and combustion. Moreover, this type of burner, through the rig, allows precise control of air and fuel proportions, thus optimizing the gaseous mixture. Another important aspect of the experimental study includes the impact on CO_2 and NOx emissions. CO emissions will decrease with increasing combustion efficiency. The purpose of the experiment with the experimental rig is to obtain precise data on how different concentrations of hydrogen and methane affect flame stability and combustion efficiency. The experimental results are expected to validate the numerical simulation model. The experimental rig and the burner were submitted for patenting, registration numbers OSIM A/00239 and A/00033 respectively.

5.3. Preliminary Results of Experimental Research

The experimental research was carried out with a burner built at a 1:1 scale compared to the calculation model from the numerical simulation phase. Both the numerical and experimental studies had the following objectives: testing combustion technology in diffusive mode; testing the evolution of combustion performance with the increase of the H_2 proportion in CH_4. The experimental tests were conducted up to an H_2 proportion of 53% (0.53) in the CH_4 mixture. The experimental program included two series: the first aimed at testing general operation, and the second at highlighting combustion performance. Prior to these two series of experimental tests, a reference operation was established by operating the burner with CH_4 only, at minimum load and unitary excess air. Against this reference flame, the effect of hydrogen presence would be highlighted.

5.4. Tests on Flame Stability for the H_2–CH_4 Fuel Mixture

The next experimental series involved the progressive increase of the H_2 proportion, with a similar increase for air, in order to determine operating conditions with a stable flame. The dosing ratio $H_2/(H_2+CH_4)$, denoted as "r", was progressively increased from 17 to 50%. The first experiment involved burning an H_2–CH_4 mixture with H_2 = 17%, with atmospheric air, serving as a reference basis for highlighting the flame evolution depending on the excess air value (a very long flame length is observed for combustion with atmospheric air). The variation of flame temperature at the thermocouple locations (t_1 at 50 mm, t_2 at 100 mm) demonstrates an increase for higher H_2 dosages, due to the faster ignition of hydrogen. The experiments highlighted the importance of excess air in the accompanying air on the combustion development, with the data for combustion at stoichiometric excess air ($\lambda = 1$) showing the highest temperature values, where Δt denotes the difference between the experimental data for $\lambda = 1.05$ and the theoretical data for $\lambda = 1$. Experimental measurements showed that as the proportion of H_2 increases, combustion occurs closer to the burner outlet, manifested by an increase in temperatures t_1 and t_2, as well as by the shortening of the flame length „ℓ".

5.5. Experimental Research on the Combustion Performance of the $\frac{H_2}{CH_4}$ Mixture

These results were based on the conclusions drawn from the previously presented experimental research, aiming to define performance parameters for H_2/CH_4 combustion and to validate the numerical simulation model. For the performance tests, the reference point for experiments consisted of maintaining a constant flame thermal power of P_t = 9.5 kW as well as a constant stoichiometric excess air value ($\lambda = 1$), while varying the H_2 fraction in the CH_4 gas mixture from 34 to 53%. As demonstrated through numerical simulation, increasing the H_2 fraction, due to its higher burning velocity compared to CH_4, led to the following conclusions about the flame: an increase in temperature at the burner outlet; a decrease in flame length. The decrease in temperature at the burner outlet with the increase of hydrogen proportion is due to the shortening of the reaction zone as a consequence of its high burning velocity in the first third of the flame. This aspect is also reflected in the temperature evolution in the mathematical model of the numerical simulation for higher H_2 proportions.

The experimental results and those obtained by numerical simulation show significant qualitative convergence. The main similarities are found in the flame length domain, the release velocity of combustion gas components, the shape of the temperature variation curves, and the value of the final temperature reached. The quantitative differences observed are explained by the different boundary conditions of the two approaches: numerical modeling was carried out in a closed environment, whereas the experiment took place in open atmosphere. This introduces additional effects in the experiment, such as heat losses and interactions with ambient air, which are not fully captured by the model. The measured temperatures constitute an essential criterion for validating the numerical simulation. The relative deviation between experimental data and simulated data is approximately 9%, a value within acceptable limits for this type of analysis, confirming the capability of the numerical model to accurately reproduce the combustion

***In research, questions are infinite, and each answer opens other paths* – Marie Curie**

Chapter 6: General Conclusions, Original Contributions and Future Research Directions

6.1. General Conclusions

The doctoral thesis entitled "***Hydrogen – an Industrial and Energy Vector for the Transition Period towards a Climate-Neutral Society***" carries out an in-depth investigation into the use of hydrogen and methane mixtures in combustion processes, aiming to evaluate the technological feasibility, energy performance, and environmental impact of this hybrid solution, in the context of the expansion of renewable energy sources (RES) and the need for their efficient integration into the existing energy infrastructure. In order to provide flexibility to RES-based systems under conditions of consumption and production variations, hybrid architectures are being developed that integrate various renewable technologies and energy storage solutions. These solutions contribute to increasing the resilience and efficiency of modern energy networks and support decarbonization objectives. The experimental component of the research was carried out on a specially designed test bench, developed in partnership with the National Research and Development Institute for Cryogenic and Isotopic Technologies – ICSI Râmnicu Vâlcea and the Politehnica University of Bucharest (UPB), being located on the UPB premises. The infrastructure was designed to simulate real operating conditions of a diffusion burner powered by variable mixtures of hydrogen and methane, with the aim of investigating combustion performance in turbulent regimes, flame stability, and pollutant emission levels. The system architecture is completely innovative, integrating constructive elements optimized for alternative fuels. Its complexity reflects a multidisciplinary approach, capable of addressing current challenges regarding decarbonization and the efficiency of thermal processes in the industrial energy sector. The experimental data obtained constitute a solid basis for validating CFD models and for formulating design and optimization strategies for burners compatible with renewable gas mixtures. The holistic approach to the combustion of H_2–CH_4 mixtures allowed for a complete investigation of the phenomena involved, starting from a critical review of the specialized literature, continuing with analytical and numerical simulations in ANSYS Fluent, and concluding with experimental validations on the dedicated test bench. This complex methodology provided a clear picture of the technical feasibility and the application potential of the proposed solutions. The main conclusions resulting from the research carried out during the elaboration of the thesis entitled "***Hydrogen – an Industrial and Energy Vector for the Transition Period towards a Climate-Neutral Society***" are: The integration of hydrogen into the energy mix represents a viable and sustainable solution for the transition towards a decarbonized energy system, with high potential for use in industry, transport, and the residential sector. Hydrogen–methane mixtures offer an efficient balance between technological innovation and compatibility with the existing infrastructure; CFD numerical modeling enabled a detailed investigation of combustion processes in a diffusion burner fueled with H_2–CH_4 mixtures, revealing homogeneous thermal distributions, high flame stability, and favorable behavior for industrial applications. The use of a mixture with 50% hydrogen proved operationally feasible; The experimental data obtained on the dedicated test bench faithfully confirmed the results of the numerical simulations, validating both the geometric configuration of the burner and the simulated operating regimes. The recorded values for flame velocity, temperature, and emissions were consistent with theoretical models; The design of the pilot burner, equipped with five gas nozzles and concave areas for air intake, contributed significantly to optimizing the fuel–air mixture and reducing pollutant formation. The diffusion combustion regime demonstrated superior efficiency in controlling NOx emissions; The injection of hydrogen into methane gas networks is technologically possible and economically justified up to a threshold of 30%, and the research results extend this limit to 50% under controlled conditions, opening real perspectives for industrial implementations; Power-to-Gas (PtG) technology and the use of green hydrogen play a central role in transforming energy systems, both through seasonal storage capacity and through integration into the conventional natural gas infrastructure; Carefully controlled experimental conditions, together with advanced instrumentation of the test bench, provided a solid platform for theoretical validation and practical testing of the proposed solutions, confirming the efficiency of combustion in turbulent-diffusion regimes; The results obtained highlight a good correspondence between numerical simulations and experimental data, especially for mixtures with 42% and 50% hydrogen, where the shape and slope of the temperature curves are similar. This correlation confirms that numerical modeling is capable of accurately capturing the fundamental physical processes of combustion, such as the localization of the thermal core and heat distribution; It was found that, with the increase of the hydrogen proportion in the mixture, higher maximum temperatures and an extension of the thermal front are obtained, reaching values of over 1900–2000°C. This behavior is consistent with the kinetic characteristics of hydrogen, which favor rapid reactions and complete combustion, consolidating the premises of its use as an energy vector in sustainable hybrid solutions; The increase of the hydrogen percentage in the mixture determines not only an intensification of the maximum temperature and an extension of the active reaction zone, but also favorable behavior regarding combustion efficiency and the reduction of incomplete emissions. Therefore, the results

obtained validate both the predictive capacity of the CFD model and the real potential of hydrogen–methane mixtures in sustainable energy applications. The research makes a substantial contribution to the development of combustion technologies adapted to alternative fuels, laying the foundations for the design of efficient, safe, and environmentally friendly burners in the context of decarbonizing the energy sector..

6.2. Original Contributions of the Doctoral Thesis

The original contributions of the thesis and its relevance in relation to the current global energy challenges are of high quality, being published in specialized journals with high impact factors, and presented at internationally indexed conferences. The innovation and importance of the research carried out within the thesis are detailed below for each chapter, with references to the author's publications, as author or co-author, thus validating the valuable contributions to the scientific community. The main elements of novelty and original contributions of the thesis entitled "Hydrogen – an Industrial and Energy Vector for the Transition Period towards a Climate-Neutral Society" are: A detailed evaluation, based on literature and recent data, of the industrial use of hydrogen and its isotopes during the period 2021–2025, focusing on the dynamics of primary energy consumption, the comparative analysis of hydrogen and isotope production technologies (including thermochemical, electrochemical, and cryogenic methods), and their integration into scenarios oriented towards the reduction of greenhouse gas emissions and achieving climate neutrality; The development of an integrated analysis of the role of hydrogen as a strategic energy vector in the transition to a sustainable energy system, by critically evaluating Power-to-X technologies and the main types of electrolysis (AEC, PEM, SOEC), complemented by the investigation of national and European potential for the production and integration of green hydrogen; An in-depth investigation of the combustion behavior of hydrogen–methane mixtures under conditions relevant for industrial applications, through the analysis of constructive configurations of burners (premix, diffusion, self-aspirating, low-NOx) and the evaluation of flame stability criteria, energy efficiency, and emissions. An integrated approach was developed, combining the theoretical fundamentals of combustion phenomenology with the modeling of turbulent jet interaction and control parameters, providing conceptual support for designing solutions compatible with the new requirements of flexibility and sustainability of hybrid energy systems; The conceptual proposal, design, and realization of an innovative diffusion burner, capable of safely operating with hydrogen–methane mixtures containing high hydrogen content (up to 50% H_2), adapted to the specific requirements of the turbulent–diffusion combustion regime; A detailed numerical modeling of the combustion process using the ANSYS Fluent platform, which included the analysis of internal flow in the combustion chamber, the distribution of velocity and temperature fields, as well as the prediction of the formation of main reactive and pollutant species. This CFD approach allowed an in-depth investigation of the phenomenology of turbulent–diffusion combustion, providing essential support for optimizing burner configuration and reducing emissions; The burner was validated through experimental testing using a specially designed test bench, equipped with measuring and control systems for monitoring combustion parameters (temperature, flame stability, emissions). This experimental stage enabled the validation of the results obtained from numerical simulations, demonstrating the consistency between the mathematical model and the real behavior of the system. Based on these results, predictive models were developed for optimizing combustion processes and reducing pollutant emissions, with direct applicability in hybrid gas–hydrogen infrastructures; A comparative analysis of the combustion process was carried out for two fuel compositions – 100% methane and an H_2–CH_4 mixture in a 50–50% ratio – under stoichiometric and excess-air conditions, in order to evaluate the influence of composition on flame stability, temperature distribution, and pollutant emission levels. The study highlighted the significant modifications of combustion characteristics generated by the presence of hydrogen, contributing to the foundation of decisions regarding the use of mixtures in hybrid installations; Two patent applications were formulated and submitted to OSIM, concerning: (1) a diffusion-type combustion device for hydrogen–methane fuel mixtures, intended for residential applications, and (2) a modular experimental stand, equipped with integrated measurement and control systems, designed for characterizing and optimizing combustion in hybrid gas–hydrogen installations. Both proposals aim at original technological solutions, with direct applicability in the context of the transition towards clean energy sources; The optimal operating conditions were established for an industrial burner powered with methane–hydrogen mixtures, by identifying the ideal combustion regime and the flame stability thresholds, depending on fuel composition and operating parameters. The results obtained provide a valuable technological guide for the safe and efficient implementation of these solutions in future industrial applications, in the context of the transition towards low-carbon fuels. The contributions brought to the development of the research field are demonstrated by the high quality and impact of the results obtained, validated through a significant number of published scientific papers: 5 articles in ISI journals ranked in Q2, 6 articles in ISI journals ranked in Q3, one article in an ISI journal ranked

Q4, papers published in ISI- and Scopus-indexed journals and conference proceedings, and 2 patent applications submitted to OSIM, as detailed in the dissemination of results section..

6.3. Future Research Directions

The large-scale integration of renewable energy sources (RES) requires a multicriteria approach for the selection and sizing of storage technologies. Hydrogen emerges as an essential energy vector, capable of reducing carbon intensity and supporting the transition towards climate neutrality. While previous estimates indicated a storage capacity of 6% of annual consumption, current data (2025) show the need for values between 10–20%. In this context, Power-to-Gas solutions based on green hydrogen become critical, especially in hybrid configurations, ensuring both short- and long-term balancing. An immediately applicable direction is the controlled injection of H_2–CH_4 mixtures into existing gas networks, gradually reducing the use of fossil fuels without major infrastructure modifications. This solution is relevant both in the residential and industrial sectors, facilitating a pragmatic and sustainable transition towards a low-emission economy. Future research directions aim to extend and deepen these solutions, in line with EU priorities on decarbonization, energy security, and technological innovation. They are presented below: Innovative solutions for reducing CO_2 emissions through the use of hydrogen and methane mixtures; Interactions between climatic and environmental factors in combustion processes; Adaptation and mitigation at regional, local, and sectoral levels; Reducing the carbon footprint through CO_2 capture and utilization; Development of efficient hydrogen production technologies; Promotion of clean energy vectors in real applications; Extension of the experimental study by testing the burner at higher powers (i.e., higher fuel flow rates – the percentages may remain the same) and identifying operating limits; Extension of the experimental study by increasing the concentration of H_2 in the mixture; Study of real-time emissions and development of automated combustion control strategies, based on dynamic regulation of excess air and exhaust gas recirculation. The aim of this approach is to reduce NO_x, CO, and unburned H_2 emissions, in accordance with increasingly strict air quality requirements; Evaluation of the possibility of integrating the burner into a smart energy system – correlated with intermittent renewable sources and Power-to-Gas technologies – can bring added flexibility and sustainability to the energy system, especially in distributed or decentralized applications; Design of modular burner configurations, adaptable to various industrial applications, such as furnaces, turbines, or boilers.

Diseminarea rezultatelor – Contribuțiile autorului la dezvoltarea domeniului de cercetare al tezei
Alina Elena Ștefănescu

Dissemination of Results – The Author's Contributions to the Development of the Research Field of the Thesis

The dissemination of the results obtained within this thesis reflects the author's significant scientific contributions to the development and deepening of the research field addressed. These contributions are supported by a portfolio of works published in internationally indexed scientific journals and presented at nationally and internationally recognized conferences. At the same time, the research activity has materialized in the registration of two patents, which attest to the applied and innovative character of the results obtained.

The publications and patents not only validate the relevance and originality of the research undertaken, but also demonstrate the author's ability to integrate the results into a broad scientific and technological framework, thus contributing to the advancement of knowledge and the potential practical valorization of these results in the addressed field.

- **Articole publicate în Jurnale ISI**
  - ✓ 1 articol publicat în UPB Scientific Bulletin (Q_4)
  - ✓ 5 articole în Q2
  - ✓ 6 articole în Q_3

1. Mihăescu Lucian; Lăzăroiu Gheorghe; **Niculescu Alina**; Pîșă Ionel; Stoica Dorel; Grigoriu Rodica-Manuela - Diffusive combustion evaluation model for [[EQUATION]] mixture with high hydrogen content, through numerical simulation and experimental validation, International Journal Hydrogen Energy, **2025**

2. Ana George, Bulubasa George, **Niculescu Alina**, Craciun, Maria, Bucur Ciprian, Ștefan Iuliana - *Characterization of water adsorption capacity at high pressure of the molecular sieve proposed to be used in TER RMSB*, Fusion Engineering and Design, vol. 215, 115039, **2025**, https://doi.org/10.1016/j.fusengdes.2025.115039

3. **Niculescu Alina**, Bulubasa Gheorghe, Ana George, Bornea Anisia - *Helium-3 Applications and Recovery Techniques*, Journal of Fusion Energy, vol. 44, issue 1, article number 20, **2025**, https://doi.org/10.1007/s10894-025-00491-6

4. Bulubasa Gheorghe; **Niculescu Alina**; Ana George; Bucur Ciprian; Crăciun Maria; Bornea Anisia - *Investigations on Hydrogen Isotope Separation Factor Employing Palladium-Based Solid Metallic Membranes*, Fusion Science and Technology, Vol. 81(4), pg. 310-314, **2025**, https://doi.org/10.1080/15361055.2024.2353967

5. Ana George; **Niculescu Alina**; Cristescu Ion; Bulubasa Gheorghe - Preliminary evaluation of NEG materials in view of CMSB replacement in HCPB TER architecture, Fusion Engineering and Design, Vol. 199, **2024**, Article number 114135, https://doi.org/10.1016/j.fusengdes.2023.114135

6. **Niculescu Alina**, Gheorghe Lazaroiu - Studies regarding the energetic properties of hydrogen and methane mixtures for domestic and industrial applications, UPB Scientific Bulletin, Series C: Electrical Engineering and Computer Science, Vol. 86 (2), pg. 383 – 397, **2024**

7. Bulubasa Gheorghe; **Niculescu Alina**; Ana George; Bucur Ciprian; Ștefan Iuliana; Crăciun Maria; Bornea Anisia - *Investigations on 3He: Hydrogen Isotope Separation Employing Palladium/Silver Membranes*, Fusion Science and Technology, vol. 80 (3-4), pg. 411 – 415, **2024**, https://doi.org/10.1080/15361055.2023.2271242

8. **Niculescu Alina**, Bulubașa Gheorghe, Ana George, Bucur Ciprian, Crăciun Maria, Bornea Anisia - *Integration of a Microchannel Reactor in a CECE Process for H2 Removal from the O2 Stream Produced by the H2 Generator*, Fusion Science and Technology, 80 (3-4), pg. 416 – 421, **2024,** https://doi.org/10.1080/15361055.2023.2273043

9. Brad Sebastian; Vijulie Mihai; Lazar Alin; Bogdan Claudia; Sirosh Oleksandr, Brill Catalin, Grafov Aleksandr; Oubraham Anisoara; **Niculescu Alina**; Bulubasa, George - *New Achievements of H2-HD-D2 Isotopic Separation with the Cryogenic Distillation Experimental Stand from ICSI Cryogenic Laboratory,* Fusion Science and Technology, Vol. 80 (3-4), pg. 455-464, **2024**, https://doi.org/10.1080/15361055.2023.2236473

10. Bornea Anisia, Ana George, Bălteanu Ovidiu, **Niculescu Alina** et. Al. - Experimental Investigation of CECE Process to Recover Tritium and Deuterium from Low Tritiated/Deuterated Liquid Waste, Fusion Science and Technology , vol. 80(3-4), pg. 365-373, **2024**, https://doi.org/10.1080/15361055.2023.2214700

11. Popescu Gheorghe; Bornea Anisia; Stefan Liviu; Ana George; Stefan Iulia; **Niculescu Alina**; Bulubasa Gheorghe; Bucur Ciprian - *Semi-quantitative determination of a tritium removal facility characteristic risk;* Fusion Engineering and Design, Vol.196, **2023**, https://doi.org/10.1016/j.fusengdes.2023.113994

12. Bulubasa Gheorghe, **Niculescu Alina**, Vasut Felicia, Ana Radu – "New method for calibration of a quadrupole mass spectrometer for hydrogen isotopes measurements" - Fusion Engineering and Design, Vol. 166, **2021**, https://doi.org/10.1016/j.fusengdes.2021.112274 ,
13. Ionete Eusebiu Ilarian; **Niculescu Alina Elena**; Spiridon Stefan Ionut; Monea, Bogdan Florian - *Magnetoresistance Behavior of Cryogenic Temperature Sensors Based on Single-Walled Carbon Nanotubes;* IEEE Sensors Journal, Vol. 21 (3), pg. 2767-2774, **2021**, https://doi.org/10.1109/JSEN.2020.3027038

- **Participări conferințe naționale și internaționale:**

1. Lucian Mihăescu, Gheorghe Lăzăroiu, **Alina Niculescu**, Dorel Stoica, Rodica-Manuela Grigoriu, Mohammed Osman – *Results of combustion test of H_2 – CH_4 mixture with high H_2 content*, paper ID: #60, 9th International Hydrogen Technologies Congress, Dokuz Eylul University, Izmir, Turkiye 25 – 28 May **2025**
2. **Niculescu Alina**, Bulubasa Gheorghe, Ana George, Bornea Anisia - *Simulation of Helium-3 Separation by Cryogenic Distillation on Experimental Facility from ICSI Râmnicu Vâlcea*, 22nd International Balkan Workshop on Applied Physics and Materials Science, Universitatea Ovidius Constanța, România, S3 P2, pg 66, Book of Abstracts, 09 – 12 iulie **2024**
3. Maria Craciun, **Alina Niculescu**, Gheorghe Bulubașa, George Ana, Anisia Bornea - Current State of Research Regarding the Hydrogen Isotope Separation by Permeation through Palladium-Based Membranes, S3 P2, pg 67, Book of Abstracts, 09 – 12 iulie **2024**
4. George Ana, **Alina Niculescu**, George Bulubașa, Ovidiu Balteanu, Radu Ana - *Tritium Extraction Processes from a Fusion Reactor Breeding Blanket*, S3 P3, pg 67, Book of Abstracts, 09 – 12 iulie **2024**
5. **Niculescu Alina Elena**, Ciprian Bucur, Gheorghe Lăzăroiu, George Ana, *Impact of Hydrogen and Methane Mixtures for Domestic and Industrial Applications under the Lens of Climate Change: A Vital Synthesis for the Energy Future*, S5 P7, pg. 95 – 96, Book of Abstracts, 09 – 12 iulie **2024**
6. George Ana, Ion Cristescu, Ovidiu Balteanu, Radu Ana, George Bulubașa, **Alina Niculescu** - *Progress in the development of the HCPB TER architecture,* 33RD Symposium on Fusion Technology, University of Dublin, Ireland, P4-130, pg. 715, Book of Abstracts, 22–27 September **2024**
7. **Alina Niculescu**, George Bulubasa, Ciprian Bucur, Iuliana Stefan, Ion Cristescu, Gheorghe Popescu - HCPB TER components performance validation, 33RD Symposium on Fusion Technology, University of Dublin, Ireland, P4-131, pg. 716, Book of Abstracts, 22–27 September **2024**
8. **Alina Niculescu**, Romulus George Ana, Ion Cristescu, Gheorghe Bulubasa - *Preliminary evaluation of NEG materials in view of CMSB replacement in HCPB TER architecture*, 15th International Symposium on Fusion Nuclear Technology (ISFNT-15), PS2-57, Fuel Cycle and Tritium Processing, Abstract-5117, pg. 443, Book of Abstracts, Las Palmas de Gran Canaria, Spania, 09 – 16 septembrie **2023**
9. Gheorghe Bulubasa, **Niculescu Alina**, Craciun Maria, Ana George, Bucur Ciprian, Bornea Anisia - *Investigations on Hydrogen Isotopes Separation Factor Employing Palladium-based Solid Metallic Membranes*, 15th International Symposium on Fusion Nuclear Technology (ISFNT-15), PS1-52, Fuel Cycle and Tritium Processing , Abstract-129d, pg. 284, Book of Abstracts, Las Palmas de Gran Canaria, Spania, 09 – 16 septembrie **2023**
10. Gheorghe Popescu, Anisia Bornea, Liviu Stefan, George Ana, Iuliana Stefan, **Alina Niculescu**, Gheorghe Bulubasa, Ciprian Bucur - *Preliminary risk analysis for a CECE-CD system at ICSI Rm.Valcea,* 15th International Symposium on Fusion Nuclear Technology (ISFNT-15), PS3-93, Safety Issues and Waste Management , Abstract-6bf1, pg. 625, Book of Abstracts, Las Palmas de Gran Canaria, Spania, 09 – 16 septembrie **2023**
11. **Alina Niculescu**, Gheorghe Bulubasa, George Ana - *Development of a Thermal Cycling Processforthe Recovery of Tritium Used in the Research Programsfrom ICSI,* XXIV the International Conference New Cryogenic and Isotope Technologies for Energy and Environment, Energen 2023, Băile Govora, Romania, TFF 19- P, pg. 329, Book of Abstracts, 18–20 October **2023**
12. Sebastian Brad, Catalin Brill, Claudia Dumitrescu, Aleksandr Grafov, Alin Lazar, Andrii Rozhentsev, Oleksandr Sirosh, Mihai Vijulie, George Bulubașa, Anișoara Oubraham, **Alina Niculescu -** New Achievements of the ICSI Cryogenic Laboratory, XXIV the International Conference New Cryogenic and Isotope Technologies for Energy and Environment, Energen 2023, Băile Govora, Romania, TFF 9- O, pg. 316, Book of Abstracts, 18–20 October **2023**
13. Gheorghe Bulubasa, Alina Niculescu - *Exploratory Studies on the Separation of Helium Isotopes Using GasChromatography,* XXIV the International Conference New Cryogenic and Isotope Technologies for Energy

and Environment, Energen 2023, Băile Govora, Romania, TFF 13- O, pg. 322, Book of Abstracts, 18–20 October **2023**

14. Maria Crăciun, Alina Niculescu, Gheorghe Bulubasa, George Ana - *Literature review on barriers against hydrogen isotopes permeation through stainless steel and EUROFER97 for use in DEMO systems,* XXIV the International Conference New Cryogenic and Isotope Technologies for Energy and Environment, Energen 2023, Băile Govora, Romania, TFF 18- P, pg. 328, Book of Abstracts, 18–20 October **2023**

15. Radu Ana, George Ana, Ovidiu Balteanu, **Alina Niculescu**, George Bulubasa - *Development of the tentative 3-D layout for the TER HCPB concept based on tritium adsorption on getter bed technology,* XXIV the International Conference New Cryogenic and Isotope Technologies for Energy and Environment, Energen 2023, Băile Govora, Romania, TFF 20- P, pg. 331, Book of Abstracts, 18–20 October **2023**

16. George Ana, Ion Cristescu, Gheorghe Bulubasa, **Alina Niculescu**, Ciprian Bucur, Iuliana Stefan, Gheorghe Popescu - *HCPB TER components performance validation,* 32nd Symposium on Fusion Technology (SOFT 2022), University of Dubrovnik, Croatia*,* P-2.256, Fuel Cycle and Breeding Blankets, pg. 748, Book of Abstracts, 18–23 September **2022**

17. **Alina Elena Niculescu**, George Ana, Gheorghe Bulubasa - *TCAP Integration in the Tritium Infrastructure of the Tritium Laboratory from ICSI RM. Valcea,* 32nd Symposium on Fusion Technology (SOFT 2022), University of Dubrovnik, Croatia, P-2.265, Fuel Cycle and Breeding Blankets, pg. 757, Book of Abstracts, 18–23 September **2022**

18. Gheorghe Popescu, Liviu Stefan, George Ana, Iulia Stefan, Alina Elena Niculescu, Gheorghe Bulubasa, Ciprian Bucur - *Semi-quantitative determination of a tritium removal facility characteristic risk,* 32nd Symposium on Fusion Technology (SOFT 2022), University of Dubrovnik, Croatia, P-2.266, Fuel Cycle and Breeding Blankets, pg. 758, Book of Abstracts, 18–23 September **2022**

- **Brevete**

1. Lăzăroiu George Cristian, Pîșă Ionel, Mihăescu Lucian, Ștefănescu (Niculescu) Alina Elena Ansamblu modular destinat dozării raportului gazelor $\frac{H_2}{CH_4}/_{aer}$ pentru controlul decarbonatării, **2025**

2. Lăzăroiu Gheorghe, Pîșă Ionel, Ștefănescu (Niculescu) Alina Elena, Negreanu Gabriel-Paul, Mihăescu Lucian, Stoica Dorel - *Modul de arzator $CH_4 – H_2$ pentru instalatiile rezidentiale dintr-un Smart City*, **2023**

- **Participări în proiecte naționale și internaționale:**

1. Agreement On Academic, Scientific and Technical Cooperation between the National Research and Development Institute for Cryogenic and Isotopic Technologies and the ITER International Fusion Energy Organization Academic, Scientific and Technical Cooperation ITER Organization CTR LGA-2024-A-149 - **2025**

2. Maximizing the Renewable Energy Hosting Capacity of Distribution networks - **2025**

3. Participarea Romaniei la EUROfusion WPBB1 si cercetari complementare / WPBB1-RO 2022 – 2024 contract nr. EU-02_03.01.**2022**

4. Participarea Romaniei la EUROfusion WPBB1 si cercetari complementare / WPBB1-RO 2024 – 2026 contract nr. EURATOM-RO/CDI/2024_001/**2024**

5. *Program Nucleu "Lab-2-Field" - Generarea de tehnologii inovative prin cercetare-dezvoltare, de la nivel de laborator la aplicație, pentru România de mâine,* Contract nr. 20N / 05.01.2023

   ✓ proiectul: PN23150105 "Tehnologii complexe de producere si stocare a hidrogenului lichid pentru aplicatii mobile" an 2023, an **2024**

   ✓ proiectul: PN23150106 „Nanostructuri 2D în fabricarea aditivă pentru energia și stocarea hidrogenului" an **2024**

   ✓ proiectul: PN 23 15 03 02 "Dezvoltarea tehnologiei inovative de separare a izotopilor Litiului prin electromobilitate şi algoritmi de inteligenţă artificială" an **2024**

   ✓ proiectul: PN 23 15 03 03 "Către un management modern al tritiului şi al materialelor asociate - Sistem modular avansat bazat pe dezvoltarea tehnologiei de separare a tritiului prin procesul CECE" an 2023, an **2024**

   ✓ proiectul: PN 23 15 03 04 "Dezvoltarea unei tehnologii de distilare criogenică pentru separarea speciilor izotopice ale hidrogenului și heliului" an 2023, an **2024**

   ✓ proiectul: PN 23 15 03 05 ''Tehnologie inovativă pentru recombinarea/arderea catalitică cu oxigenul, la temperatură joasă a izotopilor hidrogenului'' an 2023, an **2024**

6. *Program Nucleu Dezvoltare de tehnologii pentru tranziţia energetică şi impact asupra mediului – Aducând ştiinţa în scop societal – „ICSI-4EE”,* Contract nr. 9N / 07.02.2019

- ✓ proiectul: PN 19 11 01 01 "Cercetări teoretice și experimentale privind permeația simultană a izotopilor hidrogenului prin metale și barierele antipermeație" an **2022**
- ✓ proiectul: PN 19 11 01 02 "Dezvoltarea metodelor de testare a materialelor utilizate în domeniul criogeniei și a sistemelor tehnologice criogenice de purificare și separare izotopică" an 2021, an **2022**
- ✓ proiectul: PN 19 11 01 04 "Soluție inovatoare de proces CECE în scopul promovării unei noi tehnologii de decontaminare a deșeurilor lichide, slab concentrate în tritiu și de recuperare a deuteriului" an 2021, an **2022**
- ✓ proiectul: PN 19 11 01 03 "Catalizatori inteligenți pentru creșterea eficienței proceselor chimice desfășurate în prezența apei și a umidității cu aplicații în domeniul nuclear și al protecției mediului" an **2021**
- ✓ proiectul: PN 19 11 02 04 "Dezvoltarea de electroliți solizi cu conductivitate ultra-ridicată și electrozi cu stabilitate ciclică îmbunătățită pentru baterii solid-state" an **2021**
- ✓ proiectul: PN 19 11 02 05 "Nanostructuri de carbon obținute prin metoda creșterii prin depunere chimică din faza de vapori (CVD) pentru dispozitive electrochimice de producere a energiei electrice" an **2021**
- ✓ proiectul: PN 19 11 03 03 "Tehnici avansate pentru identificarea surselor de contaminare și a reacțiilor biochimice în ecosistemele acvatice" an **2021**