Doctoral Dissertation
Doctoral Program in Chemical Engineering (37th Cycle)

Hydrogen-powered aviation
A multi-scale and multi-approach investigation of fuel cell-based propulsion systems

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Summary

This doctoral research explores hydrogen-based electric propulsion for aviation, aiming to support the transition towards climate-neutral mobility systems. The work is framed within the innovation roadmap of Leonardo S.p.A., focusing on the technological readiness of hydrogen-powered proton exchange membrane fuel cells (PEMFCs) and their integration into regional aircraft platforms targeted for deployment by 2035.

The study's primary goal is to equip the company with the knowledge and tools to fully understand fuel cell technology and enhance its performance by evaluating key parameters and leveraging technological advancements.

A multi-scale and multi-approach investigation was adopted, encompassing system-level design, multi-physics modeling, and experimental validation.

At the system level, a comprehensive MATLAB-based sizing tool was developed to evaluate different propulsion architectures (fully electric and hybrid) under realistic mission profiles. The tool integrated components such as hydrogen storage, air compression, and thermal management systems, and allowed the definition of critical Key Performance Indicators (KPIs) for aircraft integration. Results confirmed the viability of hybrid configurations but highlighted significant mass penalties due to Balance of Plant (BoP) components and hydrogen storage, which are strictly linked to fuel cell efficiency.

Particular focus was placed on the comparison of different hydrogen storage options, analyzed according to KPIs such as gravimetric and volumetric densities, hydrogen release kinetics, safety, and maturity. Both physical and chemical storage methods were investigated. While physical storage solutions are more compact and straightforward in terms of system layout, chemical carriers typically require additional auxiliary subsystems—such as reactors, purifiers, and compressors—leading to increased complexity and reduced system compactness. For this reason, a detailed assessment was performed for ammonia as a representative chemical storage solution. A conceptual onboard ammonia-to-hydrogen conversion system was designed and dimensioned, including storage, cracking, purification, and thermal integration. The analysis demonstrated that, despite its lower compactness and slower hydrogen release dynamics, ammonia offers advantages in terms of safety and compatibility with existing distribution infrastructures. Performance metrics were found to be comparable to state-of-the-art physical storage solutions, highlighting ammonia's potential as a viable alternative in specific aviation contexts.

At the component level, an electrochemical model was implemented and calibrated to simulate the performance of PEMFC. This model was incorporated into system-level simulations to optimize fuel cell operation under dynamic flight conditions, in order to maximize system efficiency.

A detailed 3D CFD model of a single PEMFC was developed in ANSYS Fluent, resolving transport phenomena within the membrane electrode assembly (MEA). The model included coupled heat, mass, charge, and species transport equations, enabling the analysis of thermal hotspots, water management, and reactant utilization. Simulations provided insights into the spatial distributions of current density and temperature, informing design improvements for aviation-specific operating regimes.

The experimental campaign, conducted in partnership with Technische Universität Darmstadt, involved both *in situ* and *ex situ* characterization of PEMFCs. A wide set of membrane–electrode assemblies (MEAs) was prepared using advanced PtCo catalysts supported on high-surface-area nitrogen-doped carbon and two ionomer families: Nafion® and Aquivion™.

In situ electrochemical testing enabled the evaluation of MEA performance under different operating conditions and allowed the identification of optimal component combinations as a function of the operating regime. Among the tested materials, MEAs based on Aquivion™ ionomers and PtCo catalyst exhibited particularly promising behavior, suggesting enhanced performance potential due to improved conductivity, catalyst activity, and ionomer homogeneous dispersion.

Overall, this work delivers a robust methodological framework for the assessment and development of hydrogen-powered aircraft propulsion systems. It contributes modeling tools, experimental data, and technical evaluations that can guide future research and industrial implementation. The findings emphasize the potential of PEMFCs for regional aviation and highlight key challenges in system integration, thermal management, and materials development, offering concrete pathways to accelerate the adoption of zero-emission flight technologies.