UNLOCKING THE HYDROGEN AGE

Engineering challenges in the hydrogen value chain


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EXECUTIVE SUMMARY

Green or low-carbon hydrogen is starting to receive attention from a wide range of businesses as a potential new energy source.

Rapid changes in the global economic climate, fueled by pressures like decarbonization, decentralization, and digitalization, have spurred innovation within the energy sector and amongst heavy energy users, especially transport and industry. Organizations worldwide are implementing new energy models, based around electrification, alternative energy sources such as green hydrogen and biofuels, hydrogen for thermal engines, renewable energies for electrolysis, other technologies than electrolysis such as biomass thermolysis, and transportation of hydrogen via pipelines, trailers, decentralized energy, and platforms that enable peer-to-peer energy sharing.

Hydrogen will play an essential role in all these changes. It is an energy-dense fuel that could replace oil and gas as an energy source, especially in hard-to-electrify transport and industrial processes. Right now, most hydrogen is produced from natural gas; green hydrogen is the exception and is produced by the electrolysis of water powered by renewable energy.

In the IEA's model for Net Zero Emissions by 2050, hydrogen and hydrogen-based fuels meet 10% of global final energy demand in 2050, by which time demand will have multiplied almost sixfold to reach 530 Mt, half of which will come from industry and transport[1]. This will need to be mostly, if not all, green hydrogen – currently, only 0.49 Mt is produced by electrolysis[2].

The entire world would therefore gain from an efficient, economically sustainable green hydrogen ecosystem.

But obstacles must be surmounted to reach these ambitious goals and reap their benefits. Much of the supply chain is still being developed since green hydrogen is still very much in its infancy. Efficiency, deterioration, durability, resilience, density, and electrical power capacity are all issues that need to be addressed for the industry to be successful.

To assess, maintain, and maximize efficiency, green hydrogen will need significant infrastructure investment, including Intelligent Industry-friendly digital infrastructure and advanced digital engineering. Technology players will be strategically important to optimizing the low carbon/ green hydrogen supply chain and preparing for a safe and secure environment. Innovative ideas and best practices discovered by others must be comprehensively applied to strengthen the resilience and dependability of the hydrogen value chain.

This whitepaper explores critical engineering challenges vital to creating a low carbon hydrogen value chain and explores innovative concepts to surmount them.

Hydrogen will play an essential role in all these changes.


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GREEN HYDROGEN INDUSTRY – OVERVIEW

Key Insights

- Hydrogen is significantly more efficient than other fuel sources today and has a wide range of industrial uses, including refining, petrochemicals, and steel manufacturing.

- Green hydrogen ensures that Sustainable Development Goals (SDGs) targets such as cheap, renewable energy and resilient infrastructure are met, as well as supporting innovation.

- Declining costs of both decarbonized electricity and electrolysis technology will reduce the cost of producing green hydrogen.

- The worldwide green hydrogen market is estimated to reach $89.18 billion by 2030, with a CAGR of 54%. This is mainly due to increased demand for on-site electrolysis setups from the industrial sector.

- Only 0.1% of the hydrogen produced worldwide is green hydrogen, which is created using renewable energy.

- Europe is the market leader in green hydrogen[3].

Only 0.1% of the hydrogen produced worldwide is green hydrogen, which is created using renewable energy.

KEY ENGINEERING CHALLENGES

Companies producing green hydrogen – and their supply chain – will need to overcome significant engineering challenges to succeed in its large-scale commercialization and deployment:

1. **Plant design and return on investment**
2. **Storage of hydrogen**
3. **Transport and distribution of hydrogen**
4. **Integration of hydrogen in the development of Smart Grids**
5. **Developing hydrogen internal combustion engines**
6. **Enabling low-cost and sustainable fuel cells**

Although scaling up green hydrogen presents difficulties, contemporary digital technology and digital engineering hold many answers. Digital engineering such as digital twins, prediction models, in particular, will be crucial in finding the path to a low-carbon economy. In the rest of the paper, we demonstrate the role digital engineering plays in overcoming these challenges and explore the complexity of its application.


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ADDRESSING CHALLENGES THROUGH DIGITAL ENGINEERING

1. Using digital models to improve plant design and ROI

To meet market demand, businesses must scale up and enhance their green hydrogen plant designs. Addressing the design limitations of green hydrogen plants, the cost of alternative energy to power them, the price of desalination of water for electrolysis, and the sizing of equipment needs attention[4]. However, converting electrical energy into hydrogen via electrolysis is a rapidly advancing technology. Consequently, improving plant designs and end-to-end green hydrogen systems can be costly and complicated due to a lack of market data and maturity[5].

Digital models that simulate the operation of different technologies involved in the industrial hydrogen chain can predict the performance and costs associated with plant development and offer a promising route forward[6]. These models inform techno-economic studies that explore different scenarios to find attractive hydrogen plant cost models[7].

Building more powerful models

Capgemini Engineering, in the framework of the SISTER (Innovative Solution for Renewable Energies Storage) project, is developing a numerical tool that follows a systemic approach called THySO (Tool for Hydrogen System Optimization) that simulates the industrial hydrogen chain and considers performance, safety, cost, and environmental impact. An advantage of the THySO approach is its versatility: it can be tailored to various use cases due to a vast library of models.

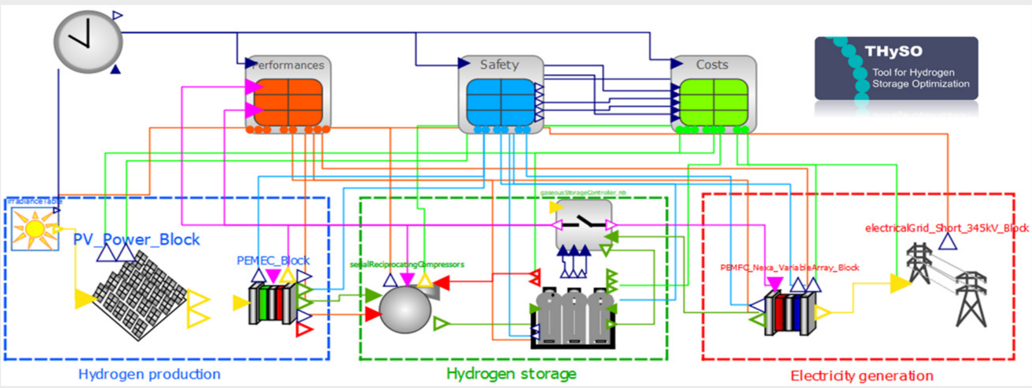


Figure 1 Example of evaluation of a Power-to-Gas-to-Power scenario using the THySO tool developed

While these economic considerations are critical, models must go further. One of the fundamental challenges of modeling the industrial hydrogen chain is the sizing of all or part of the components required in this chain according to the energy demand and the energy production capacity. In addition, models must consider the environmental impact of the hydrogen chain, such as global warming, fine particle emissions, water acidification, and eutrophication, which should all be investigated as part of the Life Cycle Assessment (LCA) of the industrial hydrogen chain[8].

Finally, massive green hydrogen plants are also being constructed inside already-existing industrial areas. This imposes additional restrictions on design to ensure that ongoing operations do not interfere with industrial green hydrogen production. So, the safety of installations using hydrogen has to be integrated into the modeling process, for instance, by simulating the risks of leakage or explosion.

2. Designing hydrogen storage tanks

Different hydrogen storage technologies have different Technology Readiness Levels (TRLs), and the usefulness of one solution over another depends on several criteria such as sizing, stationary or mobile application, duration of storage, density vs. volumetry, and environmental conditions.

- Compressed hydrogen as storage needs a large amount of energy to reach high-pressure values due to its low volumetric energy density.

- Liquid hydrogen tank materials aim to minimize heat exchange with the surrounding environment but are not made to sustain high internal pressures. However, the bigger issue is the energy to convert gas. As the liquid impacts the effectiveness and thus, the price. Along with that safety is also a big concern at high pressure.

- In the case of solid hydrogen storage, lightness, high option capacity, quick sorption kinetics, strong thermodynamic stability, and good cyclability are desired features for storage materials, and they must also be reasonably priced.

Solid storage offers a wide range of material and design options - carbonaceous porous nano-materials, metal-organic frameworks (MOFs)[9], covalent organic frameworks, complicated chemical hydrides, clathrates, amides, zeolites, and metal or intermetallic hydrides are the principal materials used. The choice of storage materials can impose restrictions like low gravimetric storage density (typically less than 10 wt%), poor reversibility, and low energy efficiency due to the substantial heat exchange that can occur during tank filling and emptying cycles. Storage of hydrogen as a solid must also consider concerns around temperature and pressure limits. Other factors include aspects of design, legal issues, societal problems, and high costs. The durability of low-storage materials like fiber, metals, and polymers, and the potential for chemical reactions raise safety issues. Exploring this complex design space is best done digitally.

Exploring solid hydrogen storage options digitally

For the construction of a solid hydrogen storage tank that achieves both productive energy efficiency and sustainable storage capacity, Capgemini Engineering is working on creating a numerical tool that determines the optimal materials.

A finite element model is being used to study sustainable and renewable alternative fibers for use in high-pressure vessels as a replacement for the conventional carbon fiber reinforced epoxy composite. Alternative fibres like basalt, E-glass, flax, and recycled carbon have been investigated for replacement.

Lower burst pressures are the consequence, and none of the other composites can withstand the 1400 bar minimum pressure requirement. Hybrid vessels incorporating T700S carbon fibres and alternative fibres are suggested to increase the physical, environmental, and financial performances in accordance with storage pressure and mechanical requirements. Increasing economic, the E-glass/T700S carbon hybrid vessel and E-glass vessel for 700 and 350 bar, respectively, are the best vessels. For a 700-bar storage, basalt/T700S carbon and E-glass are the best fibres in terms of environmental impact. Although T700S carbon/flax fibre composite looks to be more effective at 350 bar, T700S carbon composite remains the best contender for a 700-bar storage when it comes to vessel bulk.

3. Transporting liquid hydrogen for distribution

The current hydrogen transportation pipeline infrastructure is insufficient to fulfill future demand. Existing natural gas pipes cannot be used directly for hydrogen due to embrittlement. Even combining hydrogen with natural gas at a **6 percent** concentration by volume has a substantial impact on pipeline life. As hydrogen blending increases, the average calorific content of the blended gas falls, and thus an increased volume of blended gas must be consumed to meet the same energy needs. For instance, a 5% blending by volume of hydrogen would only displace 1.6% of natural gas demand. And this percentage changes with norms specified by the country[10]. When high-volume transmission via pipes is impossible, hydrogen is often transported as a liquid.

Transporting liquid hydrogen has two main challenges: "Boil-off" (i.e., the evaporation of cryogenic liquid fluid in the tanks, including an increase in pressure and deterioration of the quality of the gas) and "Sloshing" (i.e., fluid movement in the tanks that causes damage, risk of leakage, etc)[11].

This represents a double challenge in the digital engineering process because the two physical phenomena are linked and must be integrated into a single dynamic calculation model in the design of an optimized cryogenic tank that is both durable and secure. In addition, to accurately predict the consequences associated with the release of liquid hydrogen from the pressurized tank, complex physical phenomena such as flash boiling, air condensation, or liquid jet impingement need to be considered in the model. Furthermore, a certain quantity of hydrogen will be lost by evaporation, or "boil off," of liquid hydrogen, particularly when employing small tanks with high surface-to-volume ratios. Finally, an analysis of the risks associated with the use of liquid hydrogen must be made and addressed, given the potential to damage adjacent equipment and structures, and the possibilities of detonation due to leakage, among others.

When high-volume transmission via pipes is impossible, hydrogen is often transported as a liquid.

Modeling Hydrogen Transportation

Capgemini Engineering Thermal & Fluid team is actively researching these challenges and has developed new computational fluid dynamics (CFD) methods that can model complex flows as part of the Research and Innovation Project SIM4ENERGIES (Simulation for Energetics, dedicated tools and coupling strategies to address multi-physics problems).

4. Integration of hydrogen in the development of Smart Grid

Hydrogen can store and carry a vast quantity of energy. When transforming renewable electricity into an energy carrier for use in transportation and industry, hydrogen ecosystems provide a safe, adaptable, and environmentally friendly alternative. As an energy source, a storage medium, and a clean fuel, hydrogen has a significant role to play in the development of the Smart Grid[12].

Hydrogen's capacity to reach and integrate each area of the energy system enables renewable energy sources to be deployed and adopted to a far wider degree. Using contractual obligations, origin assurances, energy storage supplementary services for managing renewables in electricity networks, and direct blending with renewable power sources, hydrogen systems can be integrated into the electrical grid. Again, understanding the range of options and operating models is best undertaken digitally.

Capgemini Engineering is working with ENIT, leader of the MOSAHyC consortium, to develop Smart Grid experimental models to create a smart grid-type platform with several localized electrical energy sources, as well as storage elements of different technologies.

This MOZAHyC platform consists of setting up several energy sources, including hydrogen, that are coupled together by the conversion of renewable energies and storage stages.

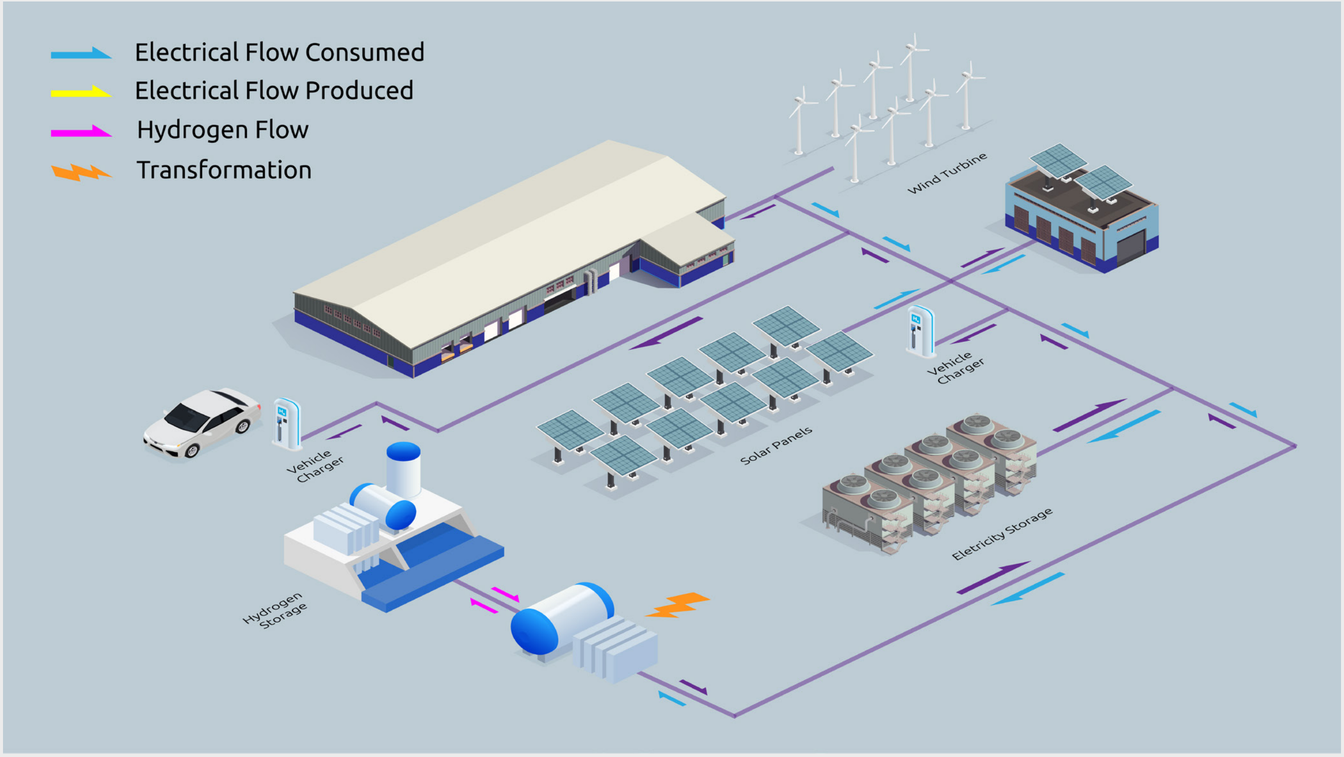


Figure 2: Production and Energy Storage network – Project MOSAHyC

5. Developing hydrogen internal combustion engines

For many in the transportation sector, reducing carbon emissions means adopting battery electric vehicles (BEVs) and fuel cell electric vehicles (FCEVs)[13]. But this doesn't mean the combustion of fuels will immediately be consigned to the engineering history books, we just need different fuels. One of these is hydrogen.

Burning hydrogen in a piston- or turbine-driven thermal engine generates no CO_2, just water and some NOx. The maturity of internal combustion engine (ICE) technology means systems can be adapted to hydrogen and other e-fuels – synthetic fuels derived from an electrochemical process – at a much lower cost than developing FCEVs.

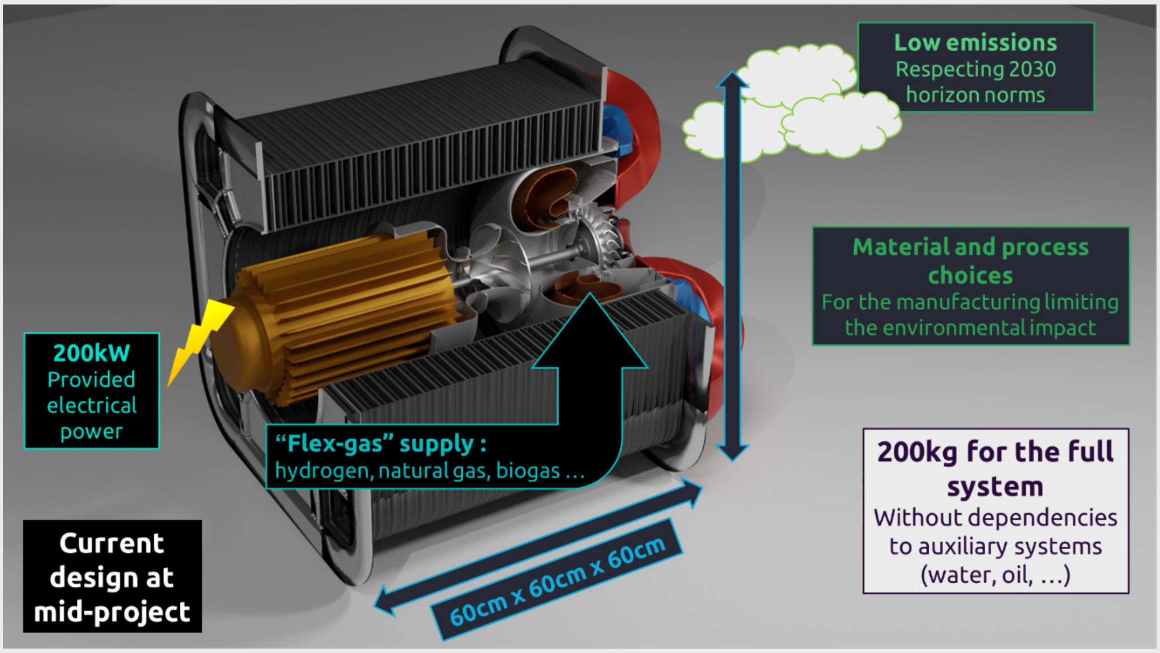
Some aspects associated with hydrogen combustion require further exploration before they can be applied extensively. The characterization of hydrogen combustion in comparison to "traditional fuels" like paraffin, natural gas, and methane is a crucial aspect. For example, flame speeds and flammability limits vary significantly with hydrogen concentration, reactant temperature, and pressure[14]. For numerical simulation, there are still gaps in the studies associated with hydrogen turbines. Furthermore, due to the high potential levels of NOX emissions, studies indicate variable levels which depend on the system configuration, geometry, and operating conditions. Moreover, security aspects will have to be explored to prevent instabilities and flashbacks. This calls for significant digital engineering work.

Hydrogen combustion engine

Technologies based on hydrogen combustion (e.g., engines and turbines) are considered complementary to fuel cells (FC) in driving the hydrogen economy. Hydrogen combustion requires lower purity levels than most FC applications and could be carried out by blending with other fuels (i.e., biomethane, natural gas, etc.), thus providing greater adaptability. However, its use in mobile applications implies several technical, economic, social, and environmental challenges.

In this context, the project HyPROPe concerns the digital prototype, test, and industrialization of an environmentally friendly "Flex-Gas" turbogenerator (using hydrogen, natural gas, biomethane, or ammonia as fuels), shown in the digital prototype developed during this project in figure 3. The target power of this system is 250 HP (Approx. 200 kW). As the main application, the microturbine is used in combination with an electric generator to power a heavy-duty hybrid truck. Other applications are envisaged (i.e., off-road, naval, and railways).

Figure 3 – Digital prototype for the HyPROPe project



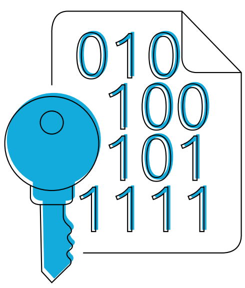
In aviation, the appropriate solution for decarbonization will depend on usage[15]. For example, electric batteries and fuel cells are a good solution for short- and medium-haul aircraft with a limited number of seats. For short-haul commuter flights, replacing original turboprops with a fuel cell and electric powertrain is a potential solution, with the possibility of using hydrogen as a fuel. For long-haul aircraft, though, the only viable option is to combust fuel, which could be sustainable aviation fuels or hydrogen.

The answer may be combining hybrid-hydrogen technology used in commercial aircraft, including propulsive systems, such as hydrogen-fueled gas turbines, hydrogen fuel cell electric propulsion, and lithium-ion batteries, but also current technology like kerosene-fueled gas turbines.

Retrofitting hydrogen propulsion

A mathematical approach called the MHyTech (Modeling Hydrogen Aircraft Technologies) is used to evaluate the feasibility of a hybrid hydrogen-powered aircraft retrofit. This tool was developed to provide insights on the potential for combining hybrid-hydrogen technology use in commercial aircraft, including propulsive systems, such as hydrogen-fueled gas turbines, hydrogen fuel cell electric propulsion, lithium-ion batteries, but also current technology like kerosene-fueled gas turbines. Investigating the most sustainable architectural configuration is one proposed optimization approach. The complete mathematical model considers the design specifications of the propulsive system and, more specifically, the decision variables, namely the engines used, the amount of fuel, and the number of proton exchange membrane fuel cell (PEMFC) and batteries (if required).

Another example is the view of a comprehensive pre-design and weight assessment methodology for electrical Vertical Take-Off and Landing vehicle (eVTOL) propulsion systems using hydrogen and batteries. Currently, over 100 eVTOL projects are under development, but the majority use batteries as power sources, reducing the mission range and autonomy.



When high-volume transmission via pipes is impossible, hydrogen is often transported as a liquid.

Hybrid hydrogen propulsion

VIABLE is a Capgemini Engineering research project that offers new solutions for Urban Air Mobility. The project develops an eVTOL based on hydrogen and batteries. VIABLE conceives an eVTOL configuration with a maximum take-off weight of 3 tons, an autonomy of 90 minutes, and a maximal mechanical power of about 1 MW. For safety reasons, the size of each power supply, consisting of the hybridization of a fuel cell and a battery, is based on degraded scenarios (for instance, the loss of one power supply).

This project proposes a methodology that includes several assets to verify the electrical hybridization concept of the power chain using fuel cells and batteries (FM2S), thermal validation of several proposed cooling solutions (SPEAC), and a weight assessment of the electrical architecture of the aircraft level (analytic weight assessment calculator).

6. Manufacturing low-cost and sustainable fuel cells

Fuel cells (FC) are one of the most relevant hydrogen systems and are key in terrestrial, naval, and, more recently, aerial mobility.

But fuel cell-based technology is an expensive and complex affair. FC systems conjure several technological constraints like high hydrogen purity requirements, lifespan, and the use of rare metals. Their energy performance is based on the stack composition, and the choice of materials composing the stack and the manufacturing method used define the environmental impact of the fuel cell[16].

Understanding their life cycle and their manufacturing process is of huge importance to enabling low-cost and sustainable fuel cells. Ultimately, this requires a multi-criteria optimization of the global process and identifying the optimal configuration possible by both reducing the environmental impacts of the process and minimizing operating costs[17]. Decision support will be necessary to identify the optimal solution(s) or to arbitrate compromises. The main challenge lies in the deployment of a methodology coupling the digital model of industrial processes and the fuel cell lifecycle digital model.

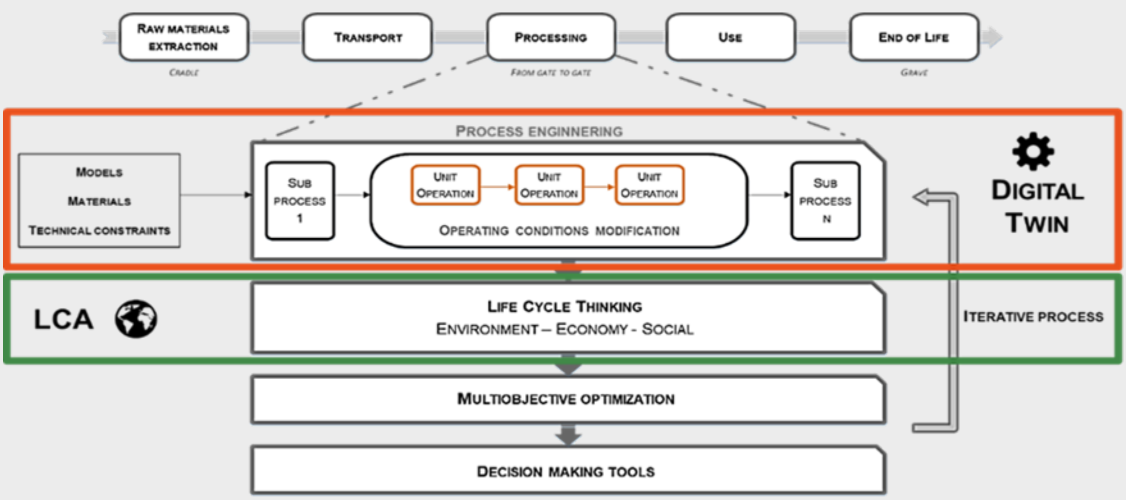
Modelling life cycle assessment of fuel-cell stack and manufacturing options

While several works have been proposed to model the Proton Exchange Membrane Fuel Cell (PEMFC) system, its complexity , due to the multidisciplinary treatment (electrochemistry, fluid mechanics, material science, etc.), limits the simulation to one part of the system, and not in totality. Apart from PEM, innovation is running on non-PEM technologies (such as alkaline, etc…) and even in PEM, on the ceramic membranes instead of existing Nafion membrane.

The work developed here, named FC-Sim (Fuel-Cell Simulation), aims to rectify this by using a multidisciplinary approach, with the coupling of modeling, simulation, and the optimization of systems, and adding sustainability as the main parameter. This multi-physics simulation of the fuel cell systems focuses on the impact of the materials for each component (e.g., the electrolyte membrane, the composition of the electrodes, the shape of the bipolar plates, etc.), and the performance of the fuel cell, considering PEMFC as the use case. The operating conditions are of particular importance, especially regarding the potential use in the aeronautical sector.

Furthermore, only a few studies have included the environmental impacts generated by the manufacturing processes of fuel cells. In parallel with previous work, the FC-Manu (Fuel Cell Manufacturing) project is about the coupling of chemical process simulation and Life Cycle Assessment methodology to develop a model representation of the actual operation of the process (i.e., a digital twin).

Figure 4 – Global methodology for the sustainable design of fuel cell manufacturing processes based on the coupling between process simulation and LCA.



CONCLUSION

The transformation journey of the hydrogen value chain: An end-to-end approach

The technology options covered in this paper illustrate the diversity and complexity of engineering choices facing stakeholders in the hydrogen value chain, who will find it challenging to resolve them all by themselves. They are point manifestations of the technology investment policies that are part of implementing an ambitious, all-encompassing transformation strategy and roadmap to convincingly create new workforce competencies, business processes, and technological capabilities, as well as coordinate a new industrial ecosystem.

To assist them in the end-to-end transformation process, from creating the transformation strategy—including business transformation—to putting the technological roadmap into practice, stakeholders should identify trusted industrial partners that, with their combined competencies, can handle the whole spectrum of capabilities needed.

Capgemini can help at all stages of the journey, from strategy to execution. With its mix of business transformation, systems integration, data science, and engineering services, Capgemini's Utilities Industry Platform utilizes digital transformation to prepare for a clean and safe hydrogen ecosystem.

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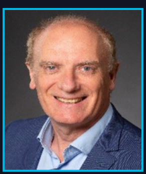

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