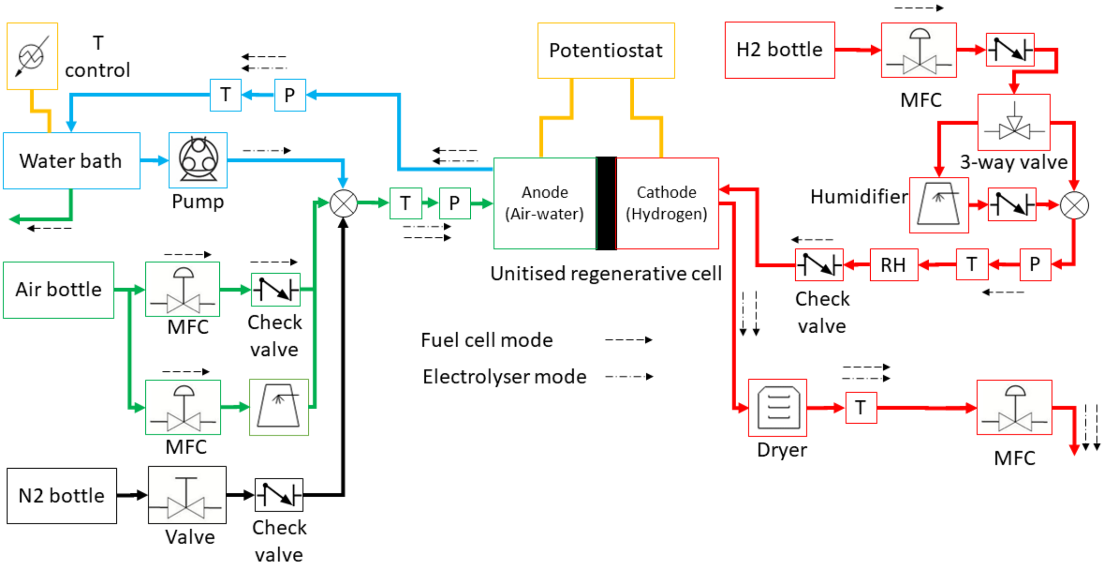
EXECUTIVE SUMMARY REPORT



Title	**Regenerative solar co-generation system**
Doc	
Issue	1
Revision	0
Date	11.12.2023
Author	Fabrizio Giordano, Saurabh Tembhurne, Sophia Haussener

Introduction

The quest for renewable energy solutions has seen significant advancements in the realm of photoelectrochemical (PEC) processes, especially in the direct conversion of solar energy and water into chemical energy. This executive summary highlights the major developments and results achieved in this project focusing on reversible Integrated Photo-Electrochemical (IPEC) devices. IPEC technology stands as a promising alternative to traditional PEC devices, effectively addressing challenges related to solid-liquid interfaces while also offering higher operational efficiencies and cost reductions.

Tandem cells, at the forefront of photoelectrochemical technology, utilize semiconductors with buried solid-state and solid-electrolyte junctions. These cells exploit smaller bandgaps, enhancing the solar spectrum response and achieving significant Solar to Hydrogen efficiencies. However, these systems are not without challenges, such as operational instability and photocorrosion at the semiconductor-electrolyte interface. Despite extensive research, a material excelling in all key aspects remains elusive.

To address these issues, our research pivoted to an innovative integrated photo-electrochemical device concept that merges photoactive and electrochemical components. This integration enables high energy and power densities, bypassing the limitations of semiconductor-electrolyte interfaces. Concentrated solar irradiation has been used to increase efficiency and reduce reliance on expensive materials like catalysts and light absorbers. This approach, however, brings its own complexities, such as elevated temperatures affecting component performance, necessitating a comprehensive understanding of heat transfer, charge transport, fluid flow, and reaction kinetics within the device.

Our contributions include developing a detailed 2-dimensional multiphysics model to simulate these complex behaviors and creating a lab-scale prototype. This prototype demonstrated a solar-to-hydrogen efficiency of 17.12% at high current densities, marking a significant step towards a commercially viable device. The culmination of this effort is a product-scale pilot which has been demonstrated for terrestrial applications with solar-to-hydrogen efficiency of ~ 25%.

Expanding our innovation, we ventured into developing reversible IPEC devices capable of operating in both forward (i.e. using sunlight to produce fuel) and reverse (using fuel to generate power) modes, an attribute especially beneficial for space applications. The 'Reversible and Integrated' technology in fact promises optimization of space and weight, as well as a reduction in the complexity for the energy production and its storage. These characteristics are essential for space missions. The system is extremely versatile and can generate Hydrogen and Oxygen to be used as propellent . At the same time Hydrogen and oxygen can be stored and with the reverse operating mode can provide electricity. Moreover, the

Arb garden is a cogeneration system that could additionally collect heat from sun in order to regulate the temperature of a lunar setting.

The current work aims to refine mass transport for optimal efficiency in both forward and reverse modes, carefully select high-performance components, enhance durability, and ultimately demonstrate that solar-powered technologies can compete with non-solar alternatives.

The project, executed by SoHHytec as the contractor and EPFL as the subcontractor, encompassed various work packages (WPs), each addressing specific aspects of the device's development and optimization. These included understanding mass-transport requirements, design analysis of flow plates and gas diffusion layers (GDLs), experimental testing for performance refinement, exploration of alternative materials and breadboard updates, and a life cycle analysis of the IPEC device and system. Each work package contributed to the overarching goal of developing a high-performance, sustainable, and reversible IPEC device, ensuring a comprehensive understanding and optimization of the technology for future energy solutions.

In our previous work, the reversible Integrated Photo-Electro-Chemical (IPEC) device, achieved remarkable efficiency in direct solar hydrogen production, demonstrating a solar-to-hydrogen efficiency of 20.6%. However, we identified challenges in maintaining long-term, stable operation in the reverse mode. A significant issue was the increased volume of water produced during operation, which impeded the transport of fuel (air/oxygen) to the catalytic sites. The main objectives in this work included:

- Optimizing Mass Transport: Understanding and enhancing mass transport for high efficiency and production rates in both forward and reverse modes.
- Component Selection: Selecting and matching high-performance components like photoabsorbers and electrocatalysts.
- Durability Analysis: Improving the longevity of both forward and backward mode operations to establish the technology as a viable alternative to non-solar methods.

We have analyzed the various aspects of mass transport in the reverse (i.e. fuel Cell) and forward (i.e. electrolyser) mode for reversible IPEC device building up on the concerned aspects in a unitized reversible fuel cell (URFC) device. Two major constraints were found in the architecture: a. blending of the catalyst to achieve dual functionality (the use of carbon based materials on the Oxygen electrode is not possible for durability reasons in the forward i.e. electrolyser mode), b. the need for wet-proofing the Gas Diffusion Layer for the reverse i.e. fuel cell mode.

With the initial design of the Integrated PhotoElectroChemical (IPEC) device, the dark forward mode, i.e. Electrolysis (EC) mode, was demonstrated with high efficiency (electricity-to-hydrogen efficiency of 80% and high power density of 1 A/cm^2 at 2.25 V. The reverse mode, i.e. Fuel Cell**Error! Bookmark not defined.** (FC) mode, while not limited by its efficiency (50% at 0.6 V), however suffered from mass transport limitations, leading to low power density of 75 mA/cm^2 at 0.6 V. The key aim was therefore to improve the water management in the FC mode. Indeed, when water is formed at the cathode of the cell (in FC mode), it has to flow out of the Gas Diffusion Layer (GDL) and the Catalyst Layer (CL), otherwise the pores of the diffusion layers are blocked and do not allow gas (i.e. reactant) to flow towards the CL, ultimately stopping local reaction and degrading performance. As in-situ measurements of water in the GDL and CL pores of an operating cell is not practical, the first task (WP0300) focused on modelling and optimization of the cell. The simulations aimed to guide the experimental work on choices of flow fields, operating conditions, and cathode GDL material/properties. The model solved for the governing transport and conservation equations without detailing the two-phase phenomena. Consequently, the results represented a fuel cell with no blockage of the pores while the analysis of the relative humidity allowed to identify the expected water condensation front. Different flow channel geometries (serpentine, spiral, and multichannel serpentine) as well as different operating conditions, choice of materials and geometries were investigated.

The results showed that the shape of the flow channels affected the pressure drop and the water distribution. The serpentine channel design showed the smallest pressure drop however with the disadvantage of a less uniform water concentration in the membrane. The circular shaped flow field showed a well-defined water front.

We conclude that no channel topology is outperforming the other options in all relevant aspects (pressure drop and homogeneity) and especially with respect to its ability to remove water droplets. In all the cases studied, flooding of the cell is likely to happen, requiring effective measures to remove water droplets. As water removal is likely the primary reason for performance decrease, methods for water droplet removal must go beyond flowfield optimization but also consider optimization of the operating conditions and materials involved.

Subsequently, WP0400 focuses on such operational and material aspects. Specifically, we assessed the inlet relative humidity and the change in the GDL materials, to enhance the droplet transport. The cell design was kept unchanged but versatile enough that different GDLs could be tested. Furthermore, the actual test bench was modified to allow for the control of the relative humidity. Specific protocols for the calibration of the system and the cell were designed.

The challenge for the GDL material of reversible IPEC is the inadequacy of carbon paper/cloth in FC mode for the electrode in contact with air. Therefore, titanium GDLs were investigated. As they are generally not wet proof, specific laboratory protocols were designed to coat PTFE on their surface. The coating was successful and hydrophobic characteristics were achieved.

Extensive studies of the cell's performance for varying relative humidities and GDL types were conducted and correlations between GDL permeability and performance were established. The optimization of the GDL resulted in an improvement by a factor of 2, i.e. 150 mA/cm^2 at 0.6 V, compared to the power density of the initial device design, while maintaining the same efficiency of 50% (for FC mode). Optimization with regards to the relative humidity led to improvements of 10-15%, i.e. wetter operating conditions (80% of relative humidity) were required as long as critical flooding could be suppressed. Higher operating current densities intensify the challenge of flooding.

During the test campaign, a protocol was successfully implemented allowing to switch automatically between power generation (FC) and fuel synthesis (EC) modes. This protocol was implemented in the on-sun experiments and shows stable operation.

For IPEC technology as well as in space deployments, photovoltaics remain pivotal for energy, therefore we have analysed different solar photoabsorber technologies that could improve the current design. We found that over the past decade, organic solar cells have seen impressive evolution, but their susceptibility to degradation limits their suitability for space applications. Multijunction solar cells on the other end, with a particular focus on III-V semiconductors and perovskite-silicon tandems, have shown substantial reliability in this field. 4-junction cells, in particular, have demonstrated efficiencies nearing 47%, making them strong contenders for space applications due to their broad-spectrum absorption capabilities. Perovskite silicon tandem is a very promising technology but it inherits stability concerns and is not yet a mature technology to be considered for space applications. Despite production challenges and higher costs of III-V semiconductors multijunction cells, their undeniable benefits in terms of efficiency, especially under concentrated sunlight, make them the convincing choice. Higher number of junctions allow to operate at lower currents, and hence minimize the ohmic losses, and subsequently relax the associated thermal stress.

Furthermore, we have proposed a preliminary breadboard design for a lunar arb garden, tailored for space applications consisting of :

- Solar Reflector and Assembly: This integral sub-system will be accompanied with deployment mechanisms and an active alignment system
- IPEC reactor: Functioning as a hub, the photo-electrochemical conversion reactor acts as an interface for various sub-systems. This involves the transfer of mass (gases and liquids), energy in diverse forms (such as electricity, heat, and radiation), and the transmission of data (sensor-generated information).

- Control System Electronics: This core unit, will comprise a centralized and a distributed unit.
- Fluid Management Systems: Emerging as a crucial sub-system, this component takes care of the flow of gases and fluids, adjusting flow rates and pressures.
- Thermal Control System: Maintaining temperature, especially within the IPEC, is of paramount significance. A substantial amount of heat from the IPEC can be harvested and rerouted to designated use.
- Water Source: Use water extracted from moon ice. This will require an additional process unit for ice extraction and purification.
- Enclosure for reactors: The reactor needs to be protected from extreme temperature drops during night operation

This design seeks to address the unique challenges posed by the lunar environment and represents a pioneering step toward harnessing sustainable energy on the Moon. The next stages of this work will involve rigorous and systematic review, testing, and simulations to further validate and refine the design, ultimately preparing it for real-world deployment. This endeavor exemplifies our commitment to advancing sustainable energy solutions not only on Earth but also in the exploration of space.

A lifecycle analysis (LCA) was performed for the studied reversible photo-electrochemical system, following a cradle-to-grave approach, taking into account the environmental impacts of the system resulting from all emissions coming from manufacturing, operation and disposal of the device and its components and materials.

The studied system was a scaled-up version of the reversible device studied in this work, including the necessary peripherals and solar concentrator. This system consisted of a 63.6 m^2 parabolic dish solar concentrator and an accordingly sized photo-electrochemical reactor for the production of hydrogen from water, producing 923 kg of hydrogen per year in Tabernas, Almería, Spain, over a lifetime of 25 years.

The functional unit of the study was defined as 1 kWh of hydrogen (HHV-based) produced over the lifetime of the system.

Having estimated the material inventory of such a system, the emissions resulting from the lifecycle of these materials were calculated with the OpenLCA software, using the Product Environmental Footprint database and the Environmental Footprint method. The impacts of said emissions were assessed in terms of climate change potential (gCO2eq/kWh H2) and land use. This resulted in an overall climate change potential between 8 and 26 gCO2eq/kWh H2, depending on whether material recycling is considered in the end-of-life of the system. The greatest impact in terms of greenhouse gas emissions originated in the construction materials (carbon steel, concrete, aluminium) for the parabolic concentrator and, to a lesser extent, in platinum group metals used in the photo-electrochemical reactor. It was shown that the system compares favourably with alternative green hydrogen production technologies (concentrated photovoltaics, PV + electrolysis) and has an impact which is orders of magnitude lower than hydrogen produced from steam reforming. The impact in terms of land use was mostly derived from the photoactive component of the device, as well as construction materials for the parabolic concentrator.

Finally, the system was assessed with respect to the strategic availability of its constituent materials in Europe. It was found that most of the materials used can be sourced within Europe, with the exception of platinum group metals, which are mostly available in South Africa. Other materials, such as gallium, indium and germanium, are refined in Europe from bauxite and zinc ores, which are in turn mostly imported from outside of Europe, although they are available in the continent in limited amounts.

In sum, the system was found to have lifecycle emissions comparable to or lower than other green hydrogen production routes and to be composed of materials which can generally be sourced within Europe.

Future research efforts should prioritize the refinement of existing methodologies and exploration of ways to enhance efficiency, especially in electrode fabrication and wet-proofing processes. Achieving a more optimized reversible IPEC could potentially revolutionize the efficiency of renewable energy storage systems and promote the widespread adoption of green energy solutions.

Aside from the research activity related to materials development, we believe that the design of an upscaled engineered system including reversible operation is the necessary following step to test the operability of the setup.

For the first prototype, the learnings developed in this and the previous project should be applied. Moreover an engineering analysis of the materials and design that could be used for the structure and the deployment considerations for space should be carried out.