Multiphysics Modeling of a reversible PEM Electrolyzer & Fuel Cell

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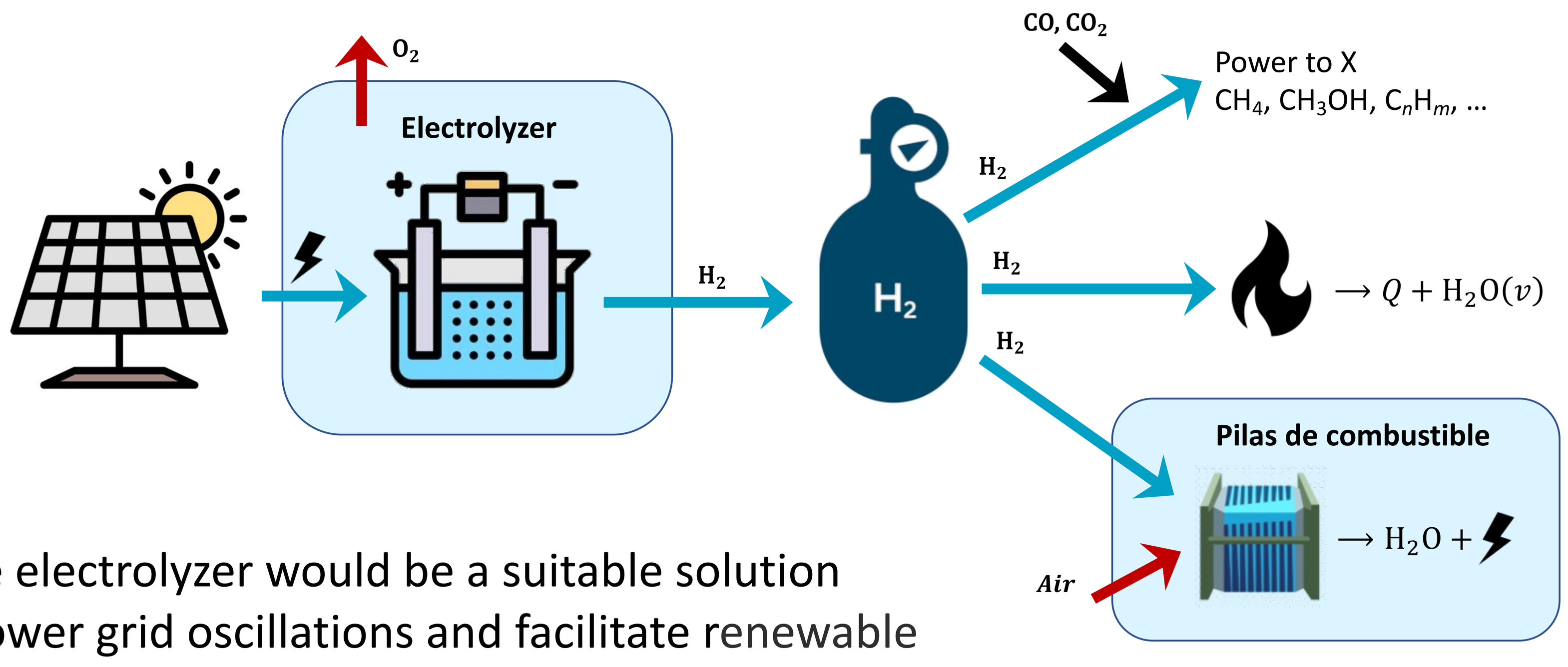
INTRODUCTION

- Electrolyzers are used to produce hydrogen and oxygen from electricity through water electrolysis. If the electricity comes from renewable sources, such as solar energy, the produced hydrogen, denoted as **green-H_2**.
- Despite often forgotten, electrolyzers also produce pure O_2, which has many different uses. E.g., in oxy-combustion processes.
- The storage and transport systems for H_2 are problematic. they require high pressures and are susceptible of leakage and other losses.
- Hydrogen Fuel Cells use H_2 to produce electricity, following the reversed operation than electrolyzers. Fuel Cells have high energy conversion efficiencies.
- Fuel Cells / electrolyzers with a polymer electrolyte membrane (PEM) are based on a cation exchange membrane that allows the transport of protons. It is possible to create a reversible device that can act as fuel cell or electrolyzer depending on the directions of the electrical and gas currents.

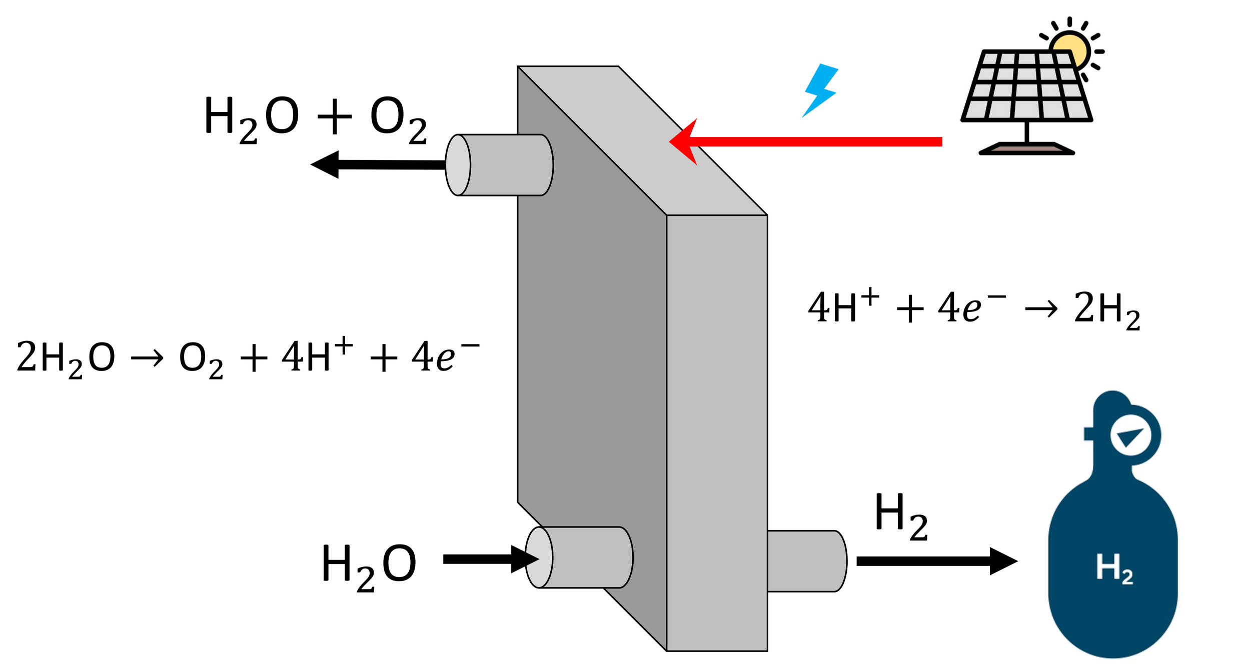
ADVANTAGES OF THE REVERSIBLE DEVICE

There are many possible used for green hydrogen. For example, Green hydrogen can be burned (as an alternative carbon-free fuel), stored and converted back to electricity using fuel cells or used as a reactant for the production of synthetic fuels or other chemicals, potentially by combination with captured CO_2.



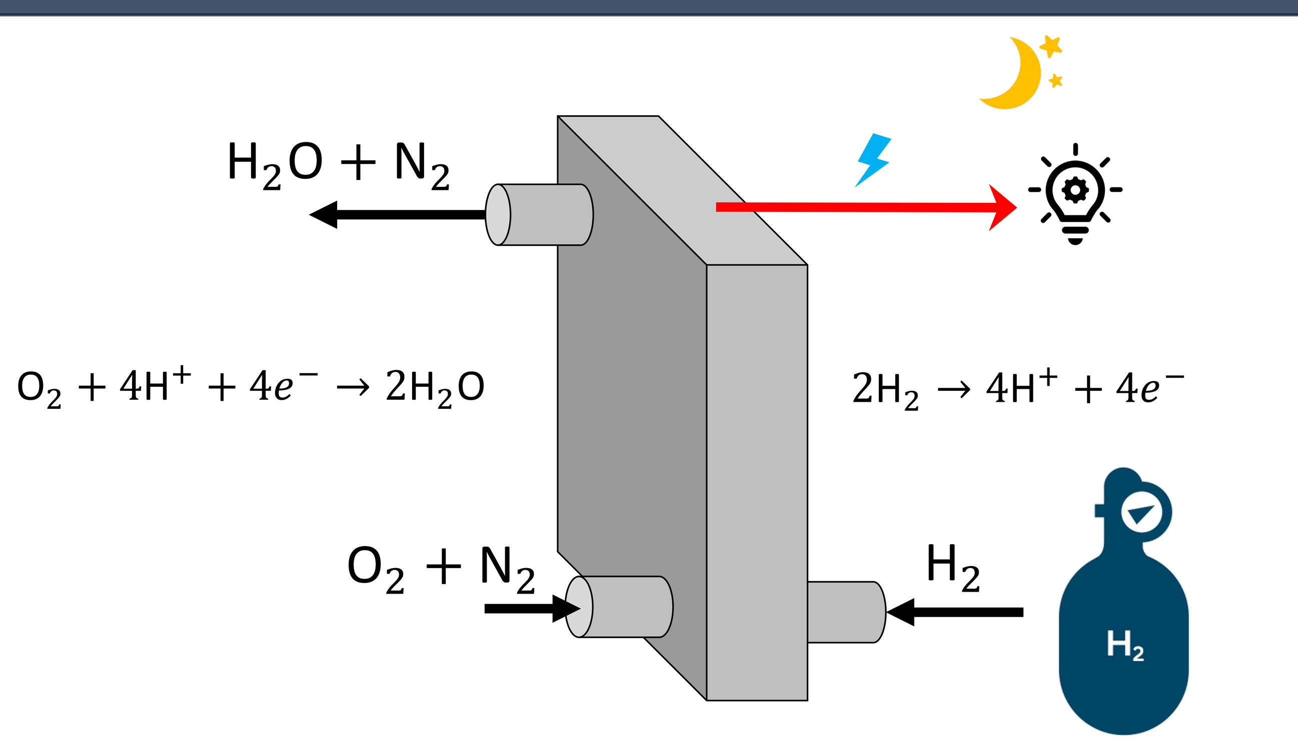
A reversible electrolyzer would be a suitable solution to buffer power grid oscillations and facilitate renewable energy integration, acting as an electrolyzer of fuel cell depending on the availability of renewable energy or the demand of electricity. This system would now only decrease the operational disadvantages of operating multiple apparatus, but also would avoid problems for long term storage and transport of the produced hydrogen.

ELECTOROLYZER CONFIGURATION



Feed with solar energy, the device produces green hydrogen and oxygen. The produced H_2 is stored for later used. Short term storage systems (normally less than 24 h) are required.

FUEL CELL CONFIGURATION

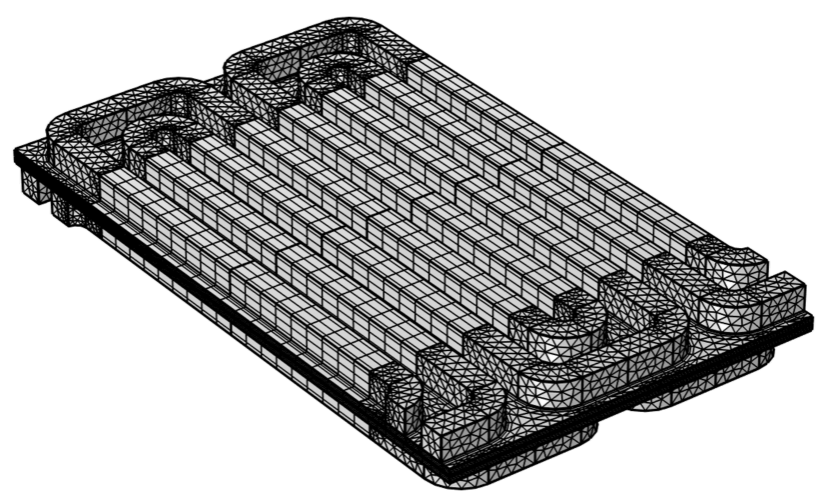


When no renewable energy sources are available (e.g., nighttime), the stored H2 is feed to de device in Fuel Cell configuration to produce electricity. The Fuel Cell can operate with O_2 from air. Therefore, the O_2 produced in the electrolyzer can be used for different applications.

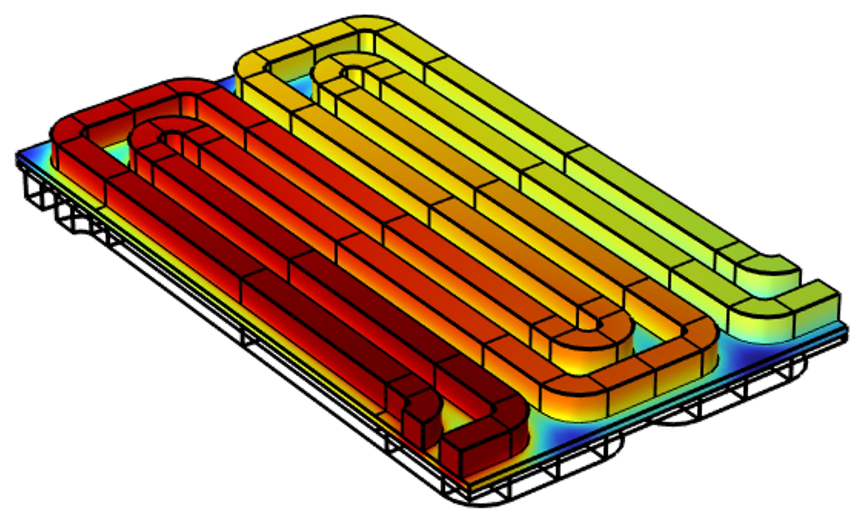
MODELING RESULTS

Modelling elements and key parameters:

- Membrane (proton exchange) 30 µm. Ideal - no cross-over transport.
- H_2 and O_2 gas diffusion layers (200 µm each). Diffusion of reactants and products from/to the catalytic layer and the flow channels.
- Thin (thickness independent) catalytic electrodes between the membranes and the gas diffusion layers.
- H_2 and O_2 gas flow channels (square channels, 800 µm width and height). Gas flow CFD model with pressure and chemical diffusion.
- Adapted 3D mesh, optimized for CFD of the flow channels, gas transport through diffusion layers, and ionic transport through the membrane.
- Fully coupled model for stationary conditions.



Detail of the geometry and the mesh



Concentration profile of H_2 within the flow channels in Fuel Cell configuration

CONCLUSIONS

A multiphysics model for a reversible PEM Electrolyzer – Fuel Cell has been implemented and solved. The model combines fluid dynamics to model the inflow/outflow of liquid and gasses: water, hydrogen, Oxygen, and Nitrogen. The model considers the relationship between the electrochemical reactions and the external electrical circuit, quantifying the electrical efficiency of the electrochemical device and the relationship with the extent of the reactions. In addition to this, the model addresses the two-directional coupling with temperature. I.e., the model includes the heat source due to activation and ohmic losses and the effect of the temperature on the efficiency of the hydrogen production.

Results show that it is theoretically feasible to use reversible electrolyzers – fuel cells devices for the efficient production and utilization of green hydrogen.

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