SOEC - Literature Review

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Objective

The aim of this project is to simulate the production of H_2 in an Solid Oxide Electolysis Cell using OpenFOAM, validated with (i) Results found by other Authors using CFD (ii) Experimental results obtained

Background

SOECs (Solid Oxide Electrolyser Cells) and SOFCs (Solid Oxide Fuel Cells) work on electrochemical principles for generating H_2 and O_2 from $H_2O(g)$ and Electrical Energy from H_2 respectively. All attempts to simulate SOEC performance have been conducted in Ansys FLUENT, using the SOEC/SOFC Module. The SOEC has a stack-like arrangement of Cathode and Anode Layers, with differing materials [1]. In High-Temperature electroysis, at operating temperatures of above 1000 K, the inlets to the cathode is hot steam, H_2O reduced to form $H_2(g)$, and O^{2-} diffuses through the cathode layer to the anode to form $O_2(g)$ which is carried through by air flowing over the anode [2].

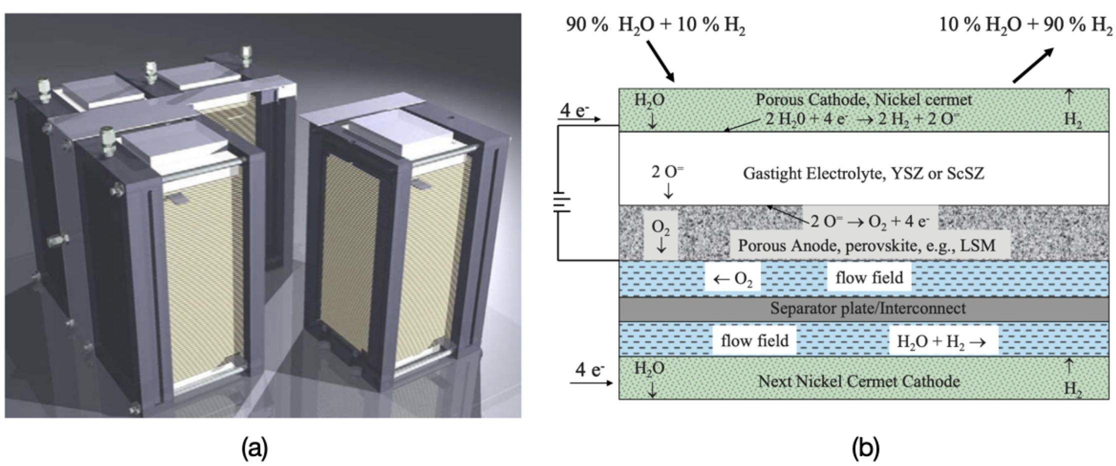

Figure 1: (a) Rendering of 60-Cell Stacks [3] (b) Electrode Cross-Section [4]

Literature

3D CFD model of a multi-cell high-temperature electrolysis stack [3]

The paper published by the Idaho National Laboratory focuses on the simulation of SOEC Performance under different parameters to validate with experimental results. The FLUENT SOFC Module, operated in the SOEC Mode was used for the simulation. This module was developed specifically for this use case, coupling mass, momentum, species and energy conservation equations.

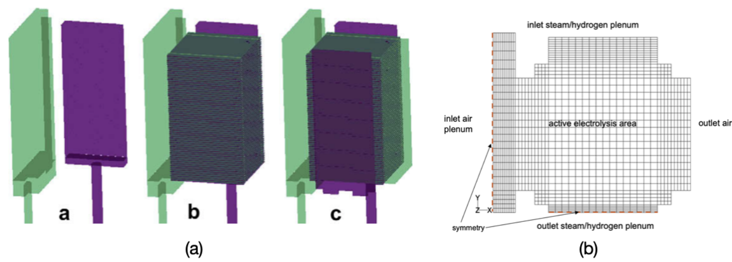

Figure 2: (a) Representation of the SOEC in FLUENT (b) Meshing used for each electrode layer

By applying different voltages (Open-Cell, 60V, 77.2V and 80V) across a 60-layer stack, the distributions of current density, temperature and H_2 and O_2 concentrations have been studied. The model developed is based on the 60-cell stack fabricated by Ceramatec Inc. Additionally, the path lines followed by the air and steam are also traced, showing recirculation throughout the stacks and inlet chamber before entering the electrode surface. The results of this paper match very well with experimental data obtained by the same INL [4], with Nickel Cermet cathode and Pervoskite anode.

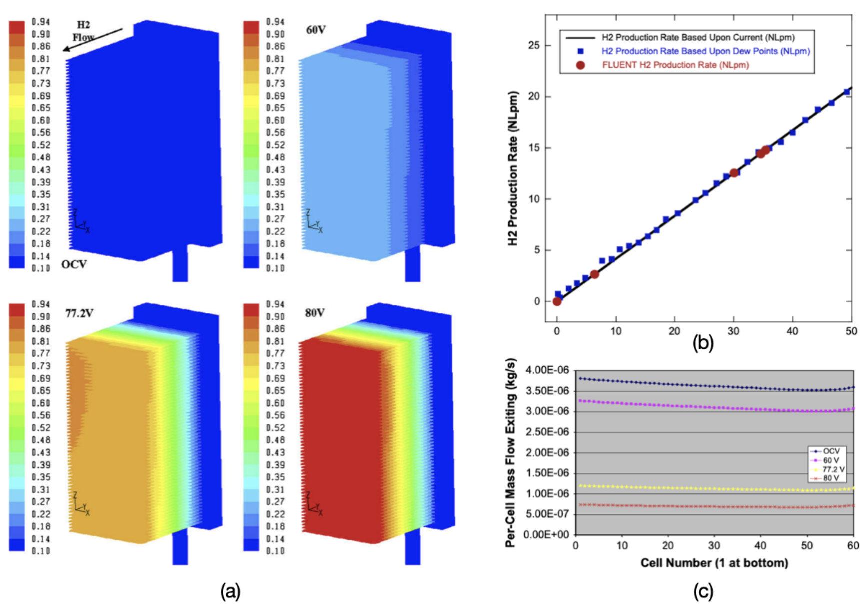

Figure 3: (a) H_2 mole fraction distribution (b) Experimental, Theoretical and FLUENT Results (c) Exit Mass Flow Rate variation with Cell Number (60-layer stack)

CFD Model of a Planar Solid Oxide Electrolysis Cell for Hydrogen Production from Nuclear Energy [5]

From the same source as before, this paper uses a 10-Cell stack for experimental validation, and focuses on the simulation of a single stack, with grid sensitivity studies giving an optimal mesh of 49392 elements. The materials used for the anode is strontium-doped lanthanum manganite (LSM), and the cathode nickel-zirconia cermet and both electrodes are graded.

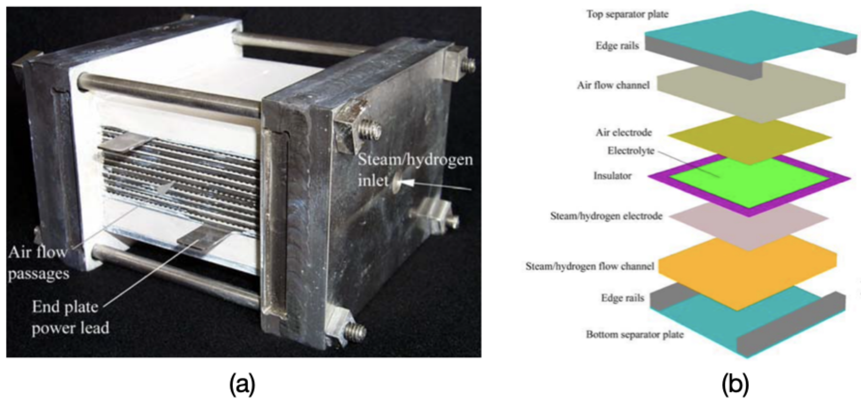

Figure 4: (a) The SOEC Stack in operation (b) The FLUENT SOFC Exploded View

The paper focuses more on mapping the current density of the experimental setup to the FLUENT model, with the constant offset explained due to the leakage of hydrogen through diffusion. Molar H_2 concentration on the electrode surface is studied, with higher H_2 content near the outlet of each electrode plate due to the advection of gas molecules with steam inlet (Steam moves from top to bottom).

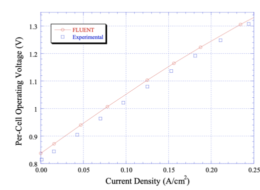

Figure 5: V-I Characteristics

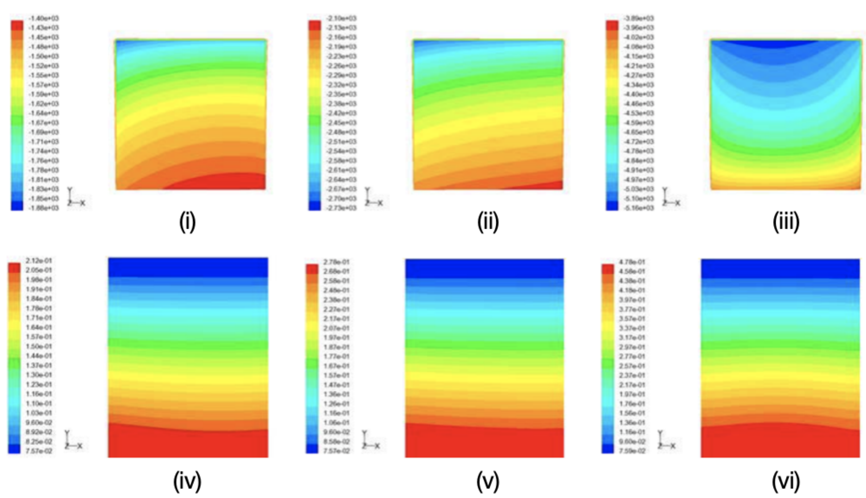

Figure 6: (i), (ii), (iii) show current density (A/m^2) for 10 A, 15 A and 30 A respectively (iv), (v) and (vi) show H_2 mole fraction for same currents

Analysis of performance optimization of high temperature SOEC... [2]

This paper's results identify key parameters affecting the hydrogen production of the SOEC, and studies the behavior of gas conversion rates with current density. Control of gas temperatures was also found to be important, because current density and hydrogen production increase with temperature, but the ions do not get enough time to permeate the electrodes, leading to slower reaction rates.

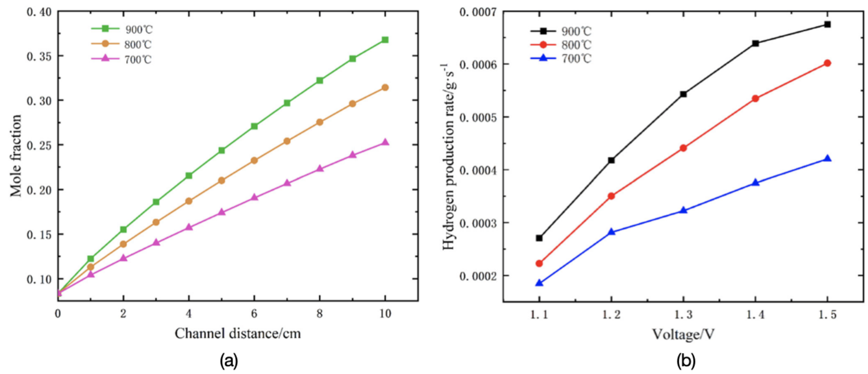

Figure 7: (a) Mole fraction of H_2 varying with channel distance
(b) Correlation between H_2 production and SOEC Voltage

Other Useful Resources

- Solid oxide fuel cells and electrolysis cells [6]: A literature review about the advantages of SOFCs and SOECs, and alternate uses in CO_2 production or carbon-fueled SOFCs.
- Review of solid oxide fuel cell materials [1] : An in-depth study about potential oxides used in SOFCs, with their desirable properties
- Electrochemical Power Sources: Fundamentals, Systems, and Applications (A textbook on H_2 usage and SOECs)

References

1. Saddam H and Li Y. Review of solid oxide fuel cell materials: cathode, anode, and electrolyte. Energy Transitions. 2020.
2. Kang C, Huaiwu P, Junfeng Z, et al. Analysis of performance optimization of high-temperature solid oxide electrolytic cell based on coupling of flow, heat, and mass transfer and electrochemistry. 2022.
3. Hawkes G, O'Brien J, Stoots C, and Hawkes B. 3D CFD model of a multi-cell high-temperature electrolysis stack. 2008.
4. O'Brien JE, Stoots CM, Herring JS, et al. High Temperature Electrolysis for Hydrogen Production from Nuclear Energy – Technology Summary.
5. Hawkes GL, O'Brien JE, Stoots CM, Herring JS, and Shahnam M. CFD Model of a Planar Solid Oxide Electrolysis Cell for Hydrogen Production from Nuclear Energy.
6. Kharton VV. Solid oxide fuel cells and electrolysis cells: selected aspects, novel materials and challenges. Journal of Solid State Electrochemistry. 2024.