Multi-Physics Modeling for Identification of Critical Factors in Solid Oxide CO_2-Steam Co-Electrolysis System Performances and Durability

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Abstract

A multi-physics modeling framework, which includes electrochemical and chemical reactions, mass transfer, and energy balance, has been developed and validated against experimental measurements to investigate the performance of solid oxide CO_2-steam co-electrolysis (SOEC) under various operating conditions and cell designs. A deep neural networks (DNN) algorithm was employed to construct reduced-order models (ROMs) according to multi-physics simulations for SOECs to systematically investigate the SOECs' electrochemical performance for both small button cell and large, 100-300 cm^2, planar cells. It was found that steam is electrolyzed with very high priority over CO_2, even if there was only small fraction of steam in the feed.

Methodology

- Numerical model SOFC-MP was applied to simulate SOECs with quasi-two-dimensional assumptions, considering three major reactions:
  - $2H_2O \rightarrow 2H_2 + O_2$
  - $CO_2 + H_2 \leftrightarrow CO + H_2O$
  - $3H_2 + CO_2 \leftrightarrow CH_4 + H_2O$
- Benchmarking with experimental measurements.

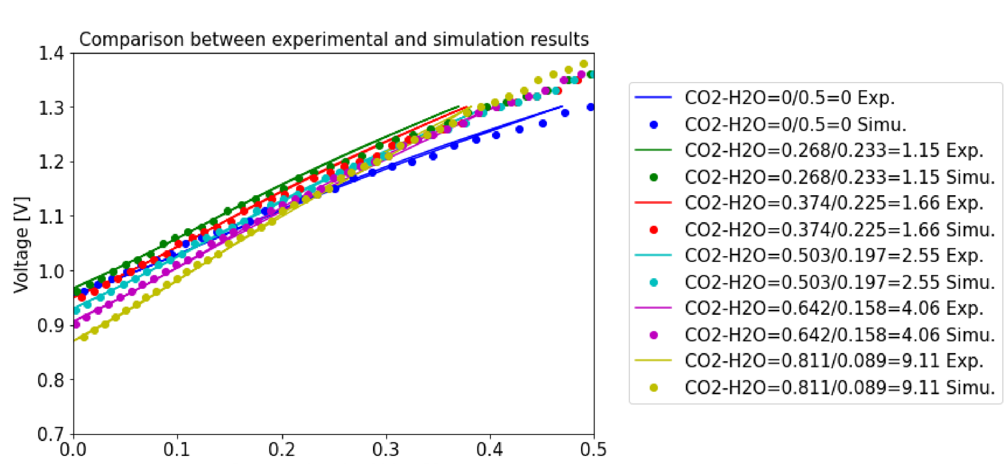

Figure 1: Comparison of voltage-current density relationships between experimental measurements and simulation results for six different fuel compositions.

- Deep Neural Network (DNN) was implemented to construct reduced-order models (ROMs) as an alternative to the numerical model to reduce computational costs.

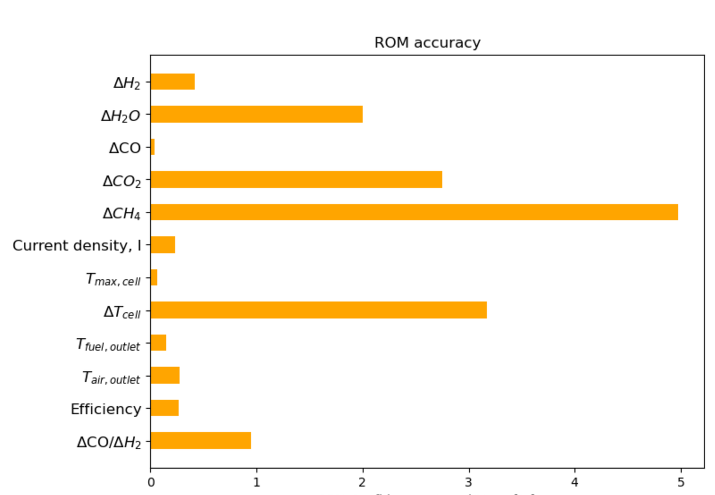

Figure 2: ROM prediction accuracies (95% confidence interval) for each electrochemical characteristics.

Results

Sensitivity studies of operating parameters

- Operating parameters' contributions to each output parameters were evaluated by DNN-ROM.
  - Current density's variation was mostly contributed by cell voltage and temperature, in percentages of 38.2% and 42.2%.
  - $\Delta CO/\Delta H_2$ ratio was highly dependent on CO_2/H_2O ratio, with a percentage of 51.64%.

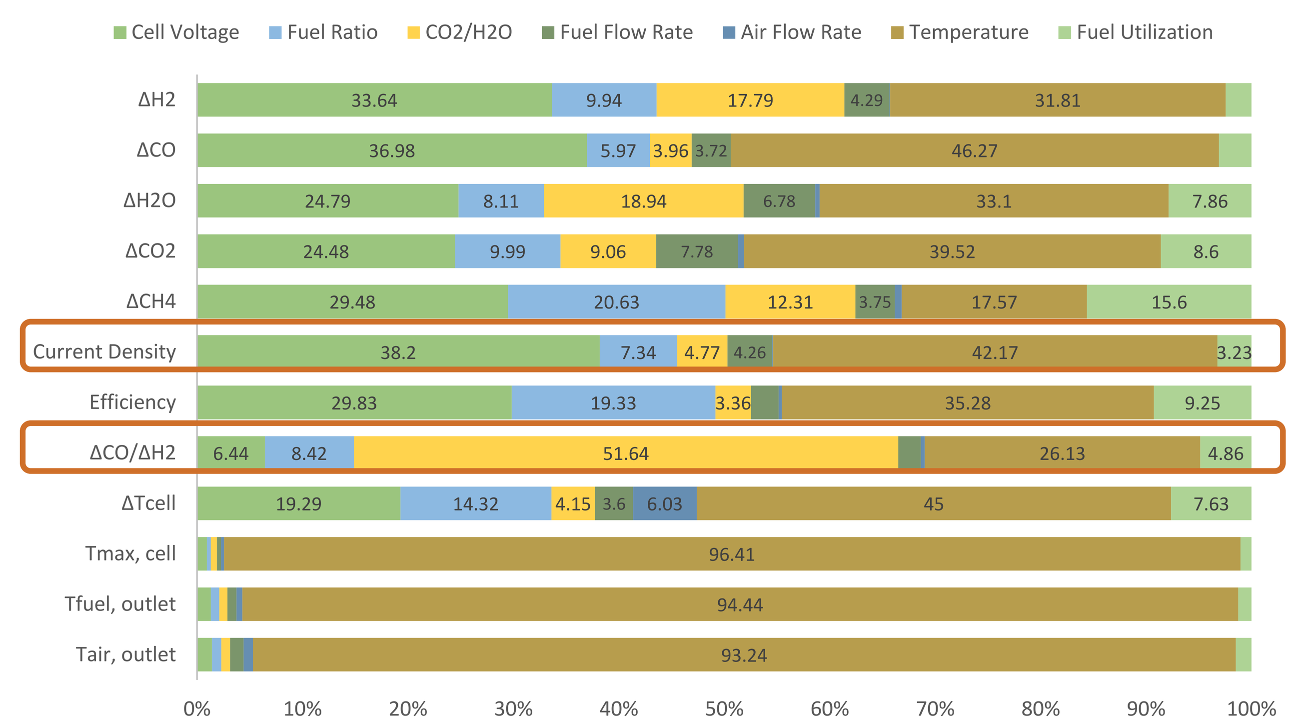

Figure 3: Influence of each operating parameter on each output in a percentage.

Sensitivity studies of cell size & thermal boundary

- Internal temperature variation showed dependencies on fuel and air flow rates with larger-size planar cells.

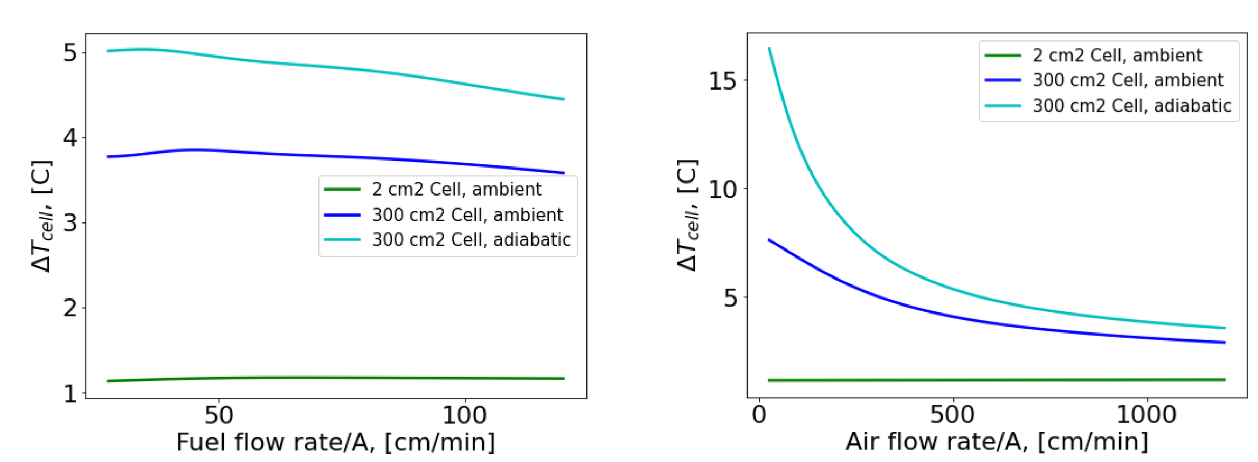

Figure 6: Comparison of cell temperature variation ΔT_{cell} among different cell sizes and thermal boundary conditions.

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Current density dependencies on temperature, cell voltage and fuel ratio

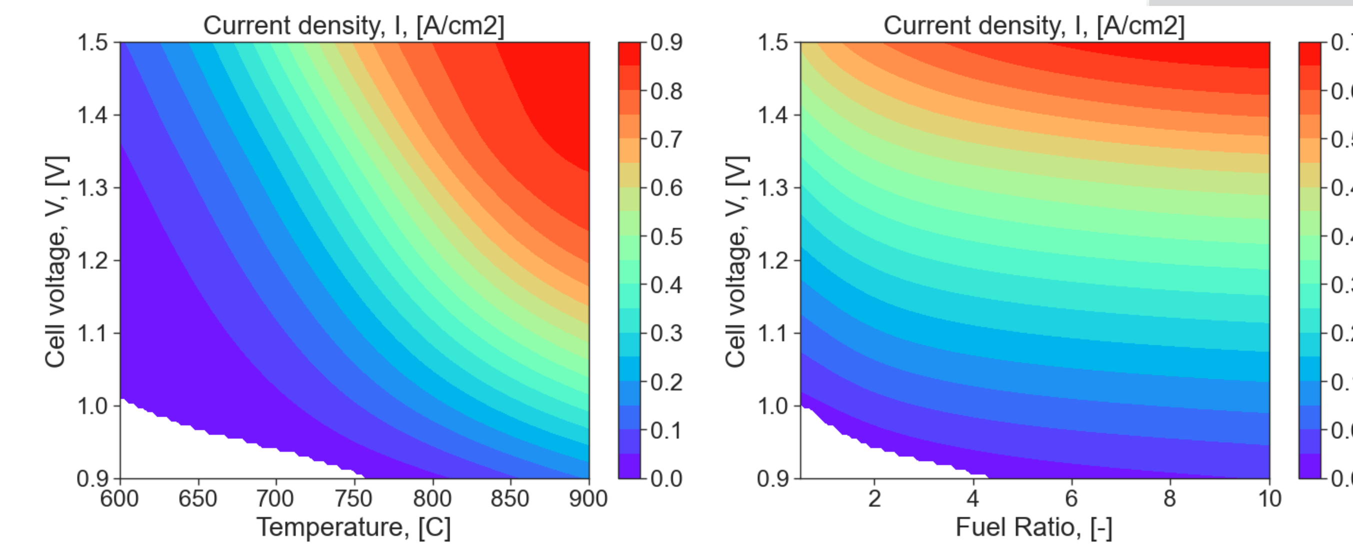

Figure 4: Current density versus temperature, cell voltage and fuel ratio.

Product ratio $\Delta CO/\Delta H_2$ dependency on CO_2/H_2O ratio, temperature, fuel ratio and cell voltage

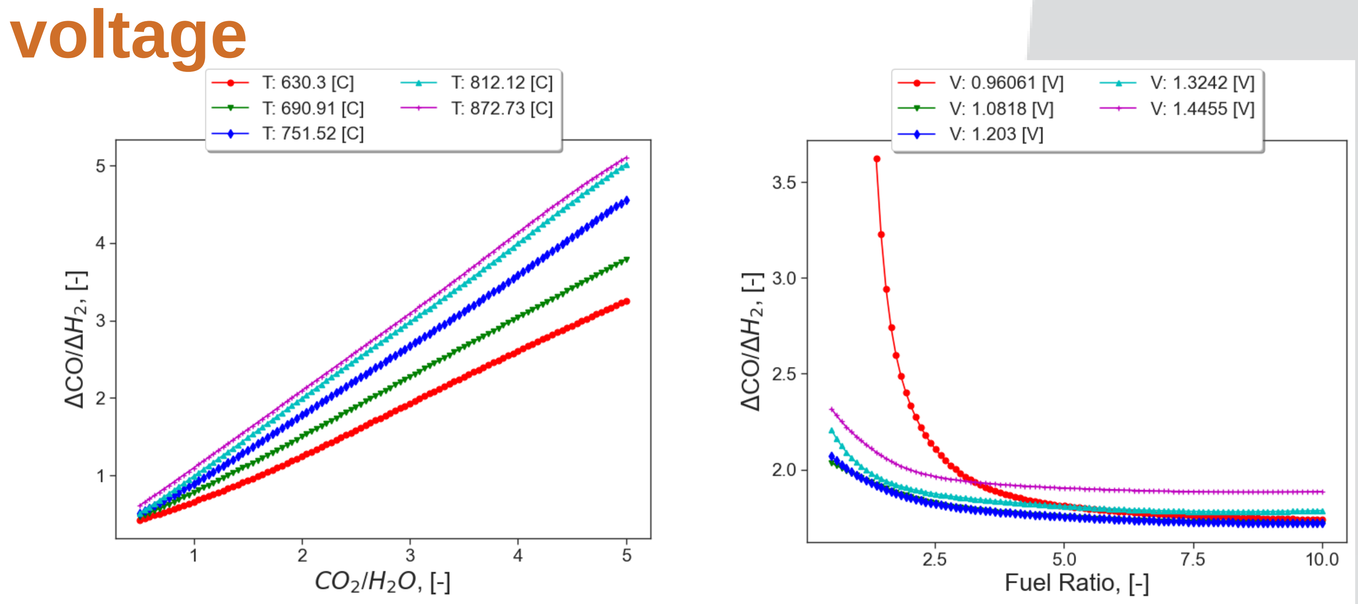

Figure 5: Product ratio versus CO_2/H_2O ratio, temperature, cell voltage and fuel ratio

Degradation & Boudouard reaction in SOECs

- Numerical model SOFC-MP has integrated several degradation mechanisms: Sr/Zr diffusion, Ni-coarsening, sulfur poisoning, and Boudouard reaction.

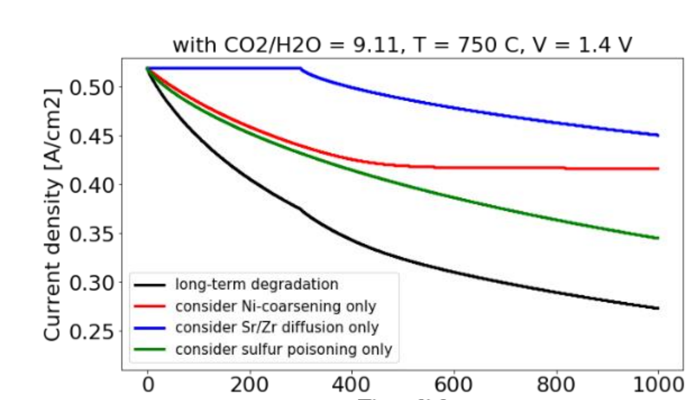

Figure 7: Different degradation mechanisms in SOECs.

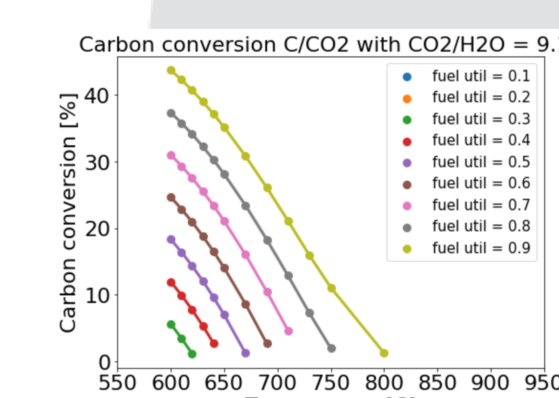

Figure 8: Carbon deposition and conversation due to Boudouard reaction.

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