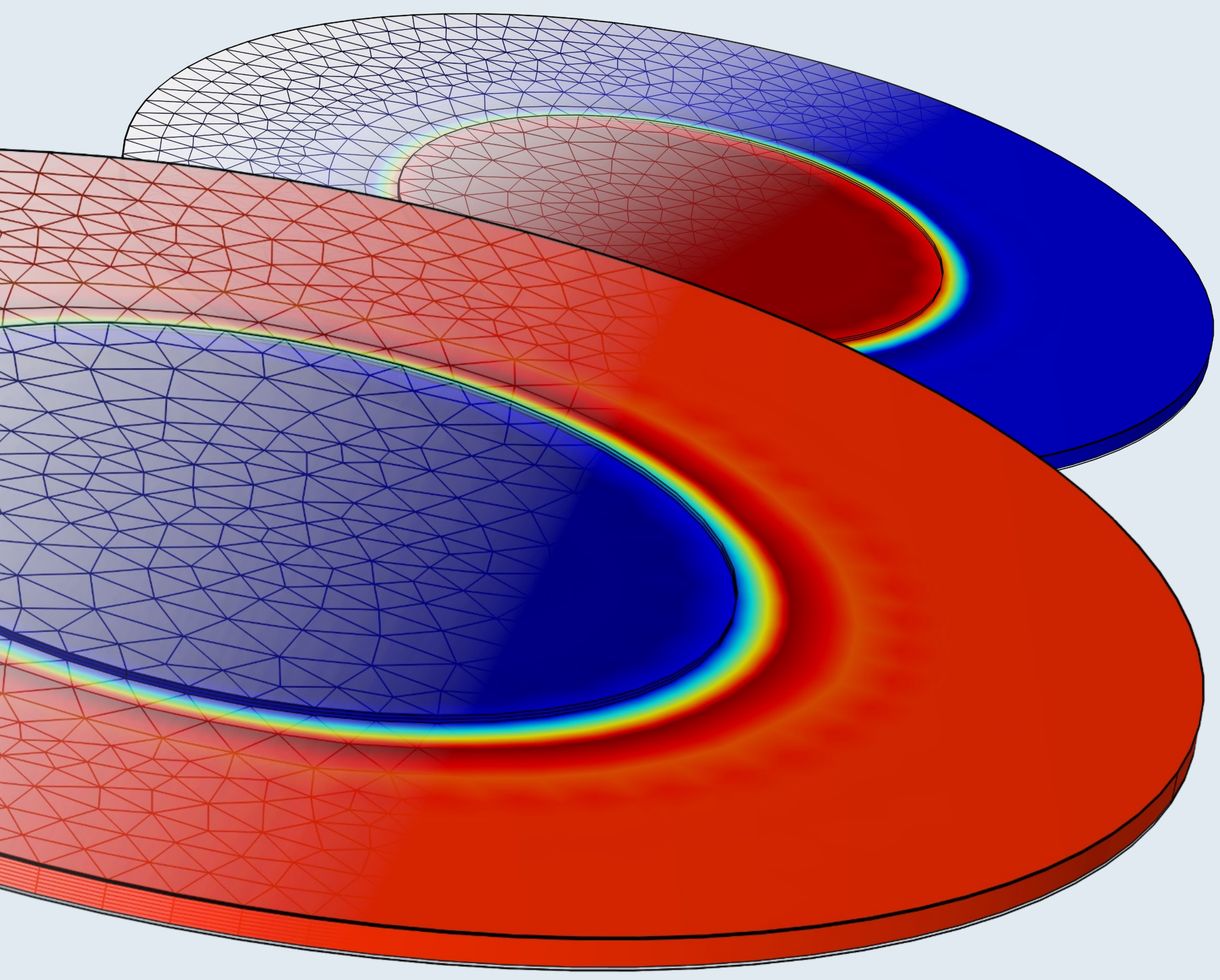

Modeling High-Temperature Electrolysis: A Multiphysics Approach

Developing a multiphysics modeling framework for high-temperature electrolysis cells to understand and mitigate electrode degradation phenomena.

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Introduction & Goals

Solid Oxide Electrolysis Cells (SOECs) are promising candidates for efficient and sustainable hydrogen production using renewably generated electricity. This is mainly due to their higher operating temperatures. Additionally, they can be integrated into Power-to-X value chains, for the de-fossilization of syngas production by the simultaneous electrolysis of water and carbon dioxide, the so-called co-electrolysis.

However, current cells exhibit life-time limitations due to degradation phenomena.
A steady-state model has been developed to elucidate the fundamentals of the electrolysis process. It considers in-cell thermodynamics, kinetics, heat transfer, chemistry, and diffusion processes. The results provide deeper insights into the occurring processes and help to elucidate the origins and mechanisms of degradation.

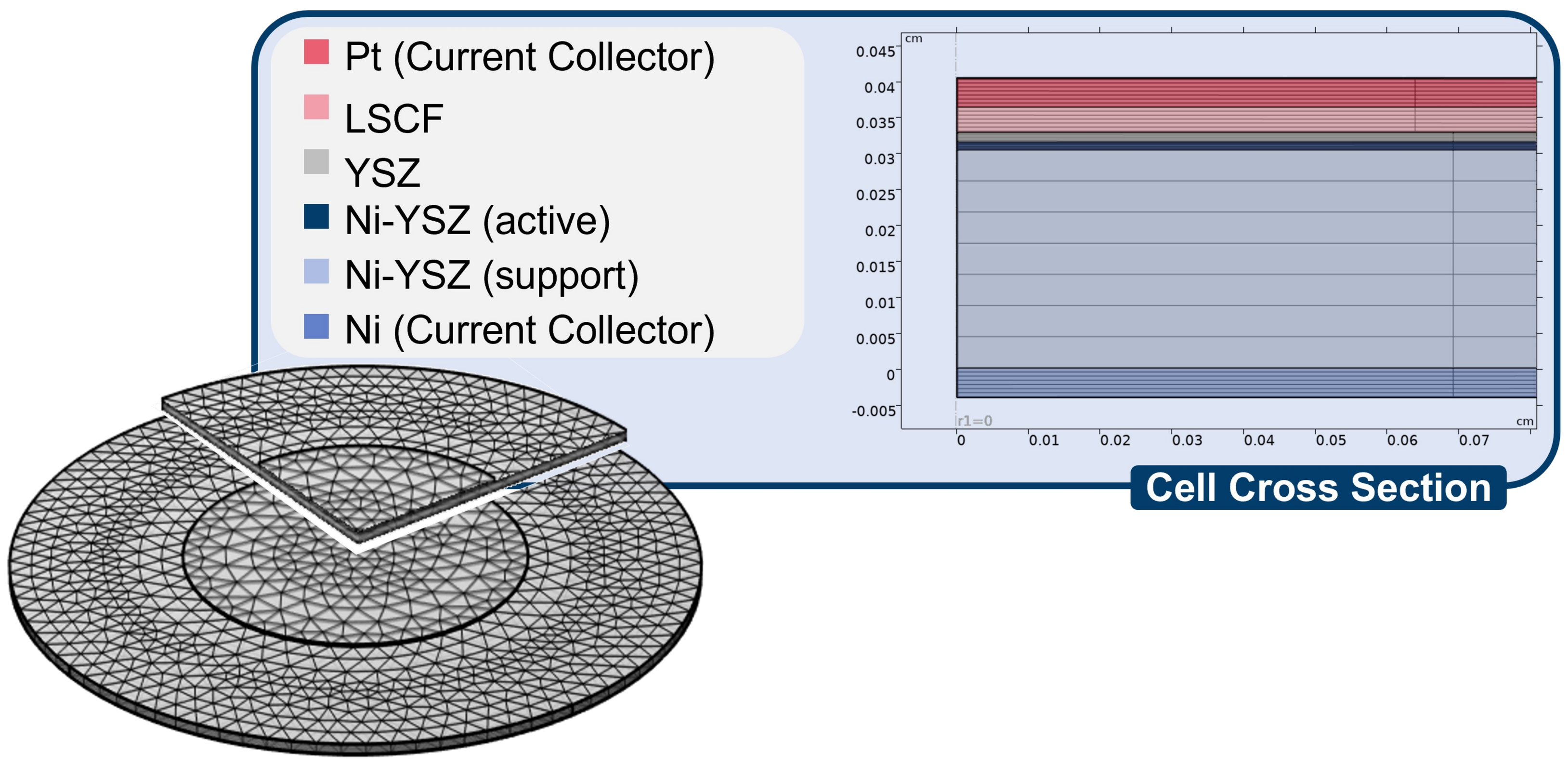

FIGURE 1: Implemented model together with the used mesh geometry and a cross section of the layer.

Methodology

Based on commercial state-of-the-art button cells, a real-scale SOEC model cell was implemented. Like the experimentally used cell, it features an (La,Sr)(Co,Fe)O_3 (LSC(F)) air electrode, an 8 mol% Y_2O_3 stabilized ZrO_2 (8YSZ) electrolyte, and a Ni-YSZ cermet fuel electrode split into functional layer and substrate.

The physical and chemical properties of each layer were modeled using the Water Electrolyzer and Chemistry modules. The model was validated using *i-V* characteristics from both the model and experimental investigations.

Results

The *i-V* characteristics and sensitivity analyses revealed that the exchange current density (i_0) matches experimental values for steam electrolysis but is an order of magnitude lower for CO_2 electrolysis. This also allows to model co-electrolysis scenarios. Meanwhile gas flow rate and permeabilities in the porous structures showed as non-sensitive parameters.

The model framework supports further research, especially on parameter variations and degradation phenomena. Time-dependent solutions can be used to study the gradual voltage increase over time.

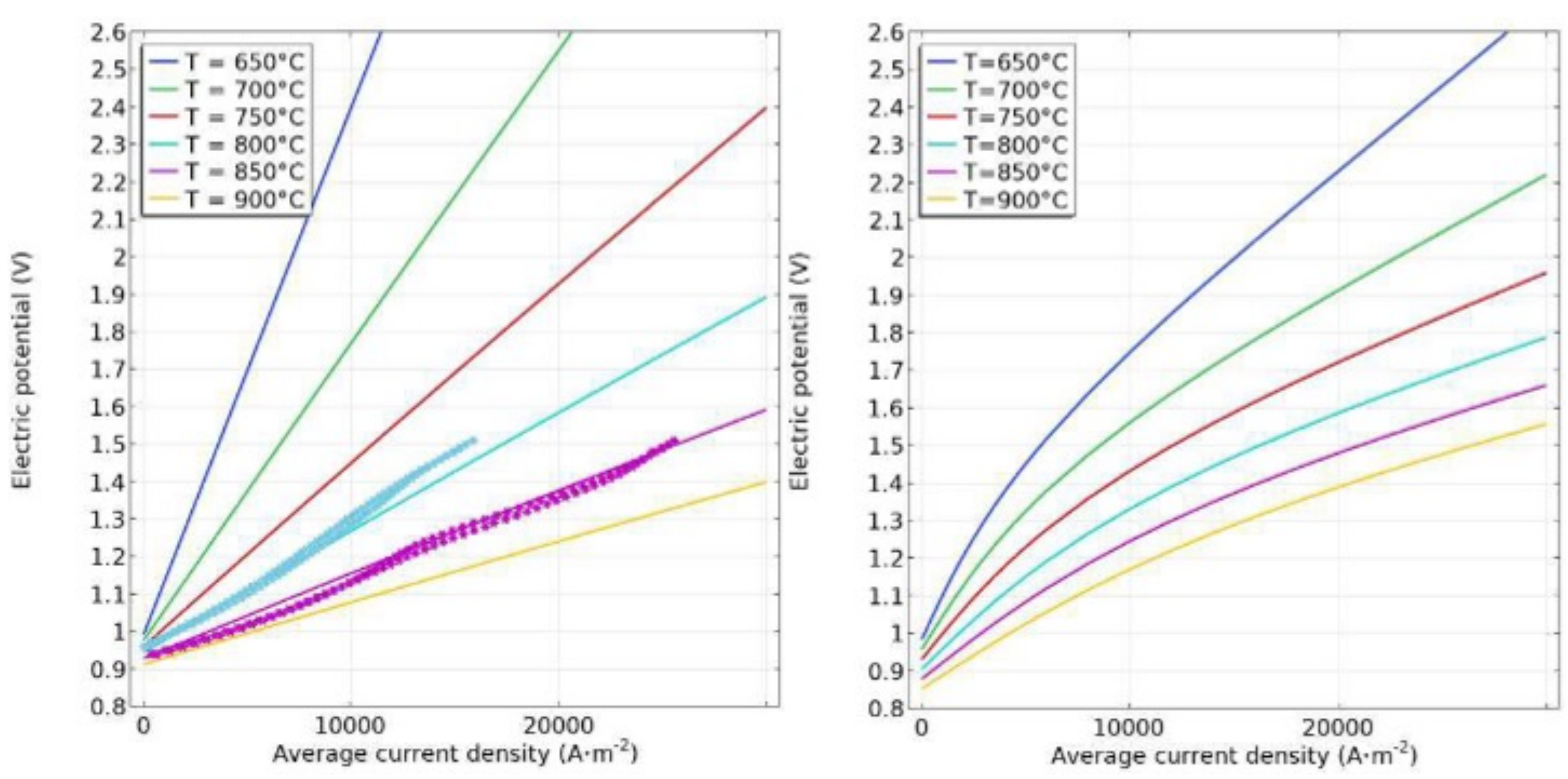

FIGURE 2: Validation results for steam and CO_2 electrolysis by comparing model results with experimental data

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