MEDIATE: A Semantic-based Material Twin and Co-Simulation Platform for Solid Oxide Fuel Cells

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The design and optimisation of Solid Oxide Fuel Cells (SOFCs) require a deep understanding of complex multiscale physical and chemical processes. Traditional physics-based models, such as finite volume and finite element methods, provide valuable insights but are computationally intensive and often rely on idealised conditions. In contrast, machine learning (ML) models enable fast and accurate predictions but require large datasets and lack interpretability. This work presents a hybrid modelling framework that integrates mechanistic models with ML techniques to enhance predictive accuracy, scalability, and reliability in SOFC performance evaluation.

A structured physical model was developed using COMSOL Multiphysics to streamline 3D and time-dependent modelling of planar SOFCs. The SOFC structure was defined in terms of fundamental physical process entities, breaking it down into reservoirs, distributed systems, and interfaces to accurately capture mass transport, electrochemical reactions, thermal dynamics, and mechanical stresses. The model topology was constructed as a directed graph, where nodes represent capacities and arcs indicate the flow of extensive quantities such as diffusion-driven mass transfer, convection, and thermal diffusion. This approach enhanced the clarity, manageability, and accuracy of the simulations while providing deeper insights into SOFC performance and degradation mechanisms under varying operating conditions. A multi-physical homogenisation framework was implemented to compute the effective properties of porous electrodes. Artificially generated cathodes and real composite anodes derived from tomography images were utilised to numerically determine effective temperature-dependent physical quantities, including electrical and thermal conductivities, permeability, and mechanical parameters (Langner et al., 2023, 2024). These effective properties were incorporated into macroscopic SOFC simulations (Makradi et al., 2025), enabling transient finite element computations to assess performance variations based on fuel cell design, operating temperatures, and electrode properties.

A Multiphysics workflow was further developed to link SOFC microstructure characteristics (e.g., porosity, tortuosity, and triple-phase boundaries) to macro-scale transport properties. Using high-fidelity COMSOL simulations, synthetic datasets were generated to train artificial neural networks (ANNs), leveraging different architectures such as Adam optimiser and Levenberg-Marquardt (Langner et al., 2024). This ANN-based approach facilitates real-time performance optimisation while significantly reducing computational costs. Moreover, the inclusion of mechanical field effects, such as creep behaviour modelled via a generalised Norton model, enables the prediction of long-term mechanical degradation mechanisms within SOFCs (Semenov et al., 2025).

A knowledge-driven simulation platform, anchored in the Elementary Multi-perspective Material Ontology (EMMO), ensures semantic interoperability and efficient data exchange across modelling domains. This ontology-based material twin framework supports SOFC design and extends electrochemical models to incorporate mechanical considerations. The software developments emerging from this research contribute to the broader goal of data-driven energy solutions by combining physics-based insights with advanced ML techniques, ultimately paving the way for sustainable, high-performance fuel cell technologies.

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