Advanced Evaluation Of Non-Precious Metal Catalysts In HT-PEMFCs Using A Three-Dimensional CFD Model

A. Samris[1], S. Mehmood[1], D. K. Bora[1], A. Faik[1]

[1]Laboratory of Inorganic Materials for Sustainable Energy Technologies (LIMSET), University Mohammed VI Polytechnic, Benguerir, 43150, Morocco

Abstract

The study addresses the challenge of improving the performance and sustainability of high-temperature proton exchange membrane fuel cells (HT-PEMFCs), which are considered a promising solution to reduce greenhouse gas emissions in heavy-duty applications such as transportation and power generation. A key issue is the development of efficient and cost-effective catalysts, particularly non-precious metal catalysts (NPMCs), to replace expensive platinum-based materials. Understanding how operating parameters such as velocity and voltage influence performance is crucial for optimizing HT-PEMFC systems.

COMSOL Multiphysics® was used to develop and simulate a three-dimensional model of an HT-PEMFC stack with 11 parallel flow channels. The model includes coupled physics phenomena such as fluid flow, species transport, and electrochemical reactions to study how different catalyst materials and operating conditions affect performance metrics like pressure distribution, hydrogen conversion, and power output.

The geometry of the fuel cell stack was created in 3D, incorporating 11 serpentine flow channels for reactant distribution. Boundary conditions were defined for inlet velocity, outlet pressure, and electrochemical reactions at the catalyst layers. Material properties were assigned for different catalyst types.

High-temperature proton exchange membrane fuel cells (HT-PEMFCs) are a promising technology for reducing greenhouse gas emissions in heavy-duty sectors such as transportation and power generation. To reduce reliance on expensive platinum-based catalysts, this study investigates the performance of non-precious metal catalysts (NPMCs) using a detailed three-dimensional CFD model developed in COMSOL Multiphysics®. The model simulates a fuel cell stack consisting of 11 parallel flow channels, accounting for coupled mass transport, fluid flow, and electrochemical reactions.

The study evaluates the effects of gas velocity, operating voltage, and catalyst type on fuel cell performance. Simulations reveal that increasing the inlet velocity enhances hydrogen conversion and leads to higher power output. A comparison between catalysts shows that the power density increases from 0.31 W/cm2 for Fe-N-C to 0.37 W/cm2 for NPMC-CNT, while the reference platinum-based catalysts Pt-Ir/C and Pt/C reach 0.44 W/cm2 and 0.46 W/cm2, respectively. These findings demonstrate the strong potential of NPMCs to approach the performance of conventional Pt-based catalysts.

This work highlights the usefulness of COMSOL Multiphysics® in evaluating next-generation fuel cell materials and optimizing system design, paving the way for cost-effective and sustainable energy solutions.

Reference

Q. Li et al., Approaches and recent development of polymer electrolyte membranes for fuel cells operating above 100 °C, Chem. Mater., 15, 4896–4915 (2003)

F. Jaouen et al., Recent advances in non-precious metal catalysis for oxygen-reduction reaction in polymer electrolyte fuel cells, Energy Environ. Sci., 4, 114–130 (2011)