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Dynamic modeling of peroxide formation in a hydrocarbon PEMFC

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Statement of the Problem: Nonfluorinated hydrocarbon proton exchange membranes (PEM) are considered as a low-cost substitute for the conventional fluorinated membrane. This replacement enhances the commercialization of proton exchange membrane fuel cell (PEMFC). Nevertheless, structural differences between fluorinated and nonfluorinated hydrocarbon membranes lead to dissimilar durability. Degradation of a PEM in a membrane electrode assembly (MEA) consists of two steps. The first step is the active hydroxyl radical formation and second is the hydroxyl radical attack the electrolyte polymer backbone. Researchers have reported models presenting the degradation phenomenon in PEMFCs working with perfluorinated hydrocarbon membranes. However, a model for investigation of degradation in a nonfluorinated membrane has not been previously studied. The purpose of this study is to develop a dynamic one-dimensional model of an MEA of sulfonated polyether ether ketone (SPEEK) that is one of the distinguished nonfluorinated PEM.

Methodology & Theoretical Orientation: The model includes gas and electrolyte phases, mass, momentum transfer by diffusion and convection intra-phase and interphases, and chemical and electrochemical reactions.

Findings: Model outputs include important chemical species concentration like feed gases, H2 and O2, water and hydrogen peroxide profiles both in gas and electrolyte phase and in various times. Two mechanisms of peroxide formation are considered in this model. One mechanism is the two electron pathway of oxygen reduction reaction, and the other is a Volmer side reaction in hydrogen oxidation reaction.

Conclusion & Significance: Results demonstrate reactant spices in both gas and electrolyte phase at different time. Accounting for solution and diffusion of the reactant spices in the electrolyte phase enable the model to predict the cross-over of these spices and consequently the hydrogen peroxide formation in the MEA. Hydrogen peroxide plays a significant role in the chemical degradation of the PEM.

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