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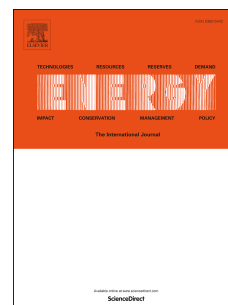
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Three-dimensional modeling of PEMFC with contaminated anode fuel

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Abstract

A novel transient multi-dimensional non-isothermal multiphase model for simulating PEMFC was developed. A multiphase agglomerate catalyst model was considered for the cathode catalyst layer, while in the anode catalyst layer the effect of CO and CO₂ presence was taken into consideration assuming two families of catalysts, Pt/C and Pt-Ru. The model predictions were compared to experimental data found in the literature and from an *in-house* PEMFC. The model was able to capture accurately the steady polarization curves of PEMFCs fed with hydrogen containing different amounts of CO and CO₂. Moreover, the corresponding transient voltage was accurately simulated. The results indicated that even low CO concentration in the anode fuel, leads to a considerable degradation of the fuel cell output current density. Among the tested gas diffusion layers, the ones with the highest thickness showed worst performance of the PEMFC. Results showed, that high tortuosity and low contact angle (hydrophobicity) of the gas diffusion layer, decreases the performance of the PEMFC.

Keywords: Numerical modeling, Anode Contamination, CO poisoning, Multiphase flow, PEMFC

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