Title: Pore-scale simulation of fluid flow through the electrodes of high temperature PEMFC using Lattice Boltzmann Method

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Abstract:

Polymer electrolyte membrane fuel cells (PEMFC) have received attention as new power sources for residential, transportation, as well as portable applications. Despite the tremendous progress in PEM fuel cell technology, namely development of the phosphoric acid doped PBI-based high temperature (> 100 ^{o}C) PEMFC with improved properties, reduced production cost, high efficiency and sufficient tolerance of Pt based hydrogen oxidation catalysts to CO impurity in hydrogen fuel (up to 2% at 180 ^{o}C) [1], degradation issues still remain. Loss of phosphoric acid by different processes, especially in high current density and elevated temperature (> 160 ^{o}C) [2], is thought to be one of the major mechanisms of degradation. Deep insight into this degradation mechanism, leading to irreversible or reversible performance loss and the relation with other degradation mechanisms and operating conditions, can come by pore-scale modelling of the mass transport phenomena, which provides detailed information at the microscopic scale.

In order to optimize the mass transport properties of the electrodes of high temperature PEMFC, firstly, the microstructure of a fiber-based gas diffusive layer (GDL) and a carbon-supported catalyst layer (CL) are reconstructed. Concerning GDL, two different commercial materials are considered and investigated by 2D Scanning Electron Microscopy images: woven GDL (Toray Graphite Paper, TGPH-120, BASF Fuel Cell) and non-woven GDL (Freudenberg Plain H2315, Freudenberg Non-wovens Technical Division). Different reconstruction techniques have been developed to deal with these materials. Woven GDL has been described by a deterministic algorithm [3], while non-woven GDL by a stochastic algorithm. On the other hand, in case of the catalyst layer reconstruction, different degrees of clustering have been investigated in order to match the actual properties of commercial materials [3].

Secondly, pore-scale flow simulations by the Lattice Boltzmann Method (PALABOS [4]) have been done to estimate the permeabilities. Rarefied gas effects are taken into account by a simplified approach, relying on a good agreement with experimental data. A model is proposed to link the permeabilities with degradation processes occurring during the high temperature PEMFC operation and, in particular, with the loss of phosphoric acid. Furthermore, the effects of the micro-morphology and the catalyst particles distribution on the durability of the electrolyte membrane are studied. Some optimization strategies are proposed in order to improve fuel cells durability.

This work is part of the on-going European ARTEMIS project, within the Fuel cells and Hydrogen Joint Undertaking (FCH-JU). The purpose of ARTEMIS is to develop and optimise alternative materials for a new generation of European membrane electrolyte assembly, while reducing cost and increasing durability.

[1] Q. Li, J.O. Jensen, R.F. Savinell, N.J. Bjerrum. *High temperature proton exchange membranes based on polybenzimidazoles for fuel cells***.** Prog. Polym. Sci. 34 (2009) 449.
[2] S. Yu, L. Xiao, and B. C. Benicewicz. *Durability Studies of PBI-based High Temperature PEMFCs*. FUEL CELLS 08, 2008, No. 3–4, 165–174
[3] U. Salomov, E. Chiavazzo and P. Asinari, *Pore-scale modeling of fluid flow through electrodes for high temperature proton exchange membrane (HT-PEM) fuel cells*, submitted to Computers and Mathematics with Applications, 2012.
[4] www.palabos.org