POLITECNICO DI TORINO
DOCTORAL PROGRAM IN ENERGETICS
Ph. D. THESIS PROPOSAL

Subject
3D Microstructure Experimental Analysis and Statistical Reconstructions of Solid Oxide Fuel Cell Electrodes with Applications to Numerical Simulations of Reacting Mixture Flows and Performance Evaluation

List of proponents (with e-mail address of the responsible person)		
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Description of the international background of the proposal

Computational modeling of fuel cell electrode/catalyst layers is an important tool in understanding the different electrochemical reactions and transport phenomena occurring within fuel cell electrodes. Proper modeling of this layer is required for an accurate prediction of cell behavior which in turn can be used for the development of more efficient fuel cells.

In macroscopic CFD approaches such layers are typically modeled as infinitely thin interfaces populated by sources and sinks or as very thin homogeneous porous layers. However, these layers are neither infinitely thin nor homogeneous and, thus, modeling in this fashion leads to a loss of information about the microstructure and its varying effects on the reacting mixture flows which pass through and into the structure. Thus, the utility of relying only on such macroscopic representations limits the general applicability of these macroscopic models as tools for design and for predicting fuel cell performance over a wide range of conditions. Furthermore, such macroscopic models cannot aid in the design of the electrode/catalyst layer itself. In order to address this latter point, a microscopic/mesoscopic modeling approach can be used, e.g., the Lattice Boltzmann Method (LBM), which models the reacting mixture flow through the porous microstructure of the electrode/catalyst layer. However, to do so requires reconstructing the porous geometry of this layer which can be done by using 2D microscopic images of cross-sections of the layer to generate 3D geometries from, for example, stochastic models which are relatively cost efficient and lead to similar structures with approximately the same characteristics of porosity, catalyst loading, three-phase boundaries, etc. as the original structure.

Unfortunately a quite wide set of the 3D reconstruction methods exist, which mainly depend on the accuracy (i.e. the number of statistical moments considered by the regression) of the applied technique. Moreover previous experience on using this kind of techniques is based on different application fields (mainly environmental engineering and underground physics), which may lead to improper conclusions for fuel cells, because the peculiar features of involved porous media are drastically different.

Research program objectives (intermediate and final) and expected results

The research program can be divided in four steps.

- Experimental characterization of microscopic topology by means of 2D BSE–SEM (back scattered electrons due to scanning electron microscope) and EDS–SEM (energy dispersive spectrometry due to scanning electron microscope) image of SOFC electrode/catalyst layer.
- Statistical numerical reconstructions based on different techniques, which are systematically compared with the original experimental picture in order to evaluate the reliability of the statistical regression.
- Numerical simulations of the fluid flow of reactive mixtures in the reconstructed topologies.
- Comparison of the numerically estimated performance with the actual global performance measured in the DENER–LAQ laboratory dealing with SOFC technology in terms polarization curve and electrochemical properties.

The expected result of the proposed project is to develop a complete analysis process starting from the microscopic experimental characterization of the SOFC materials up to the final user–level performance. This goal is part of ongoing collaboration project with Virginia Polytechnic Institute VTECH.

List of publications of the proponents and/or specific references (with titles)

[1] Asinari P., von Spakovsky M. R., Cali' Quaglia M., Kasula B. V., Direct numerical calculation of the kinematic tortuosity of reactive mixture flow in the anode layer of solid oxide fuel cells by the Lattice Boltzmann Method, Journal Of Power Sources, ISSN: 0378-7753, (in press).

[2] Asinari P., Asymptotic analysis of multiple-relaxation-time lattice Boltzmann schemes for mixture modeling, Computers & Mathematics With Applications, ISSN: 0898-1221, (in press).

[3] Asinari P., Semi-implicit-linearized multiple-relaxation-time formulation of lattice Boltzmann schemes for mixture modeling, Physical Review E, Statistical, Nonlinear, And Soft Matter Physics, vol. 73, pp. 056705-1-056705-24, ISSN: 1539-3755, 2006.

[4] Asinari P., Viscous coupling based lattice Boltzmann model for binary mixtures, Physics of Fluids, vol. 17, pp. 067102-1-067102-22, ISSN: 1070-6631, 2005.

[5] Asinari P., Cali' Quaglia M., von Spakovsky M. R., Kasula B. V., Numerical simulations of reactive mixture flow in the anode layer of solid oxide fuel cells by the Lattice Boltzmann method, Proceedings of ESDA 8th Biennial ASME Conference on Engineering Systems Design and Analysis, vol. 1, pp. 1-15, ISBN/ISSN: 0-7918-3768-8, 2006.

[6] Asinari P., Coppo M., von Spakovsky M. R., Kasula B. V., Numerical simulations of gaseous mixture flow in porous electrodes for PEM fuel cells by the lattice Boltzmann method, Proceedings of III International Conference on Fuel Cell Science, Engineering and Technology, vol. 1, pp. 93-102, ISBN/ISSN: 0-7918-3757-2, 2005.

[7] Asinari P., von Spakovsky M. R., Cali' Quaglia M., Kasula B. V., L. Mercado, 3D Microstructure Reconstructions of Solid Oxide and Proton Exchange Membrane Fuel Cell Electrodes with Applications to Numerical Simulations of Reacting Mixture Flows using LBM, submitted to ASME Conference, 2007.