Simulation of the Structure of Proton-Exchange Membrane Fuel Cell by Microlevel Cellular Models

Nazariy Jaworski, Uliana Marikutsa, Ihor Farmaha, Volodymyr Karkulovskyy

Lviv Polytechnic National University <u>nazariyjaworski@gmail.com</u>.

Polymer electrolyte membrane or proton exchange membrane fuel cells (PEFC) provide a potentially clean and portable source of power. This is of major interest to the transport industry as well as for power generation at fixed sites.

PEFC structure is complex in general case and can't be modeled by geometric primitives. Microlevel cellular models can be used to consider such structural inhomogeneities. They describe complex structure in a form of representative volume elements (RVE) that are three dimensional matrices of voxel-cells [1]. Cells contain scalar intensities conditionally in the range from zero to one. The components of composition are defined by subdiapasons of those intensities. When the number of cells is big enough, models can adequately describe such types of composites as composites with disperse filler, fibrous filler, mutually permeable components, functionally-graded components, laminates and all of their combinations. There are five main structure construction methods that can build described types of structures [1, 2]: scalar random field construction; random ellipsoid particles construction; random Bezier curve based fibers construction; random transition layers construction.

Typical cell components within a PEFC stack include [3]: the ion exchange membrane; an electrically conductive porous backing layer (also referred to as gas diffusion layers or current collectors); an electro-catalyst (the electrodes) at the interface between the backing layer and the membrane; cell interconnects and flowplates that deliver the fuel and oxidant to reactive sites via flow channels and electrically connect the cells. The polymer membrane is sandwiched between two sheets of porous backing media. In intimate contact with the membrane and the backing layer is the catalyst layer.

Fig. 1 shows the microlevel cellular model of the proton-exchange membrane fuel cell, structure of which is the combination of laminate,

CADMD 2018, October 19-20, 2018, Lviv, UKRAINE

fibrous filled and mutually permeable structures. To build such complex multicomponent model one should apply construction methods as follow:

- generate scalar random field in the middle of RVE that corresponds to microporous catalyst layers of the fuel cell;
- iteratively generate random Bezier curve based fibers with different length and radius under and over random field, which correspond to gas diffusion layer of the fuel cell;
- generate solid layer in the middle of RVE that corresponds to membrane.



Fig.1 Microlevel cellular multicomponent structural model of proton-exchange membrane fuel cell.

Such microlevel model can be used in FEM simulation of physical processes within fuel cell to achieve more precise results because it provides detailed structural features.

References

- N. Jaworski, I. Farmaga, and U. Marikutsa. "Building the Micro-Level Composite Materials Structure Models in the Problems of their Optimal Design." *Scientific Bulletin of UNFU*, 25.8:359-366, 2015.
- [2] N. Jaworski, I. Farmaga, U. Marikutsa, "Random transition layers construction method and its application in heterogeneous structures multiscale modelling by OpenCL technology". *Bulletin Lviv Polytechnic National University "Computer sciences and information technologies"*, 826: 385-394, 2015.
- [3] USDE, "Fuel Cell Handbook," 7th Edition, EG&G Technical Services, Inc., Morgantown, U.S. Department of Energy, Office of Fossil Energy, National Energy Technology Laboratory, 2004.

CADMD 2018, October 19-20, 2018, Lviv, UKRAINE