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The work is submitted to the International Scientific Conference "Priority directions of development of science, technologies and equipment", Italy (Rome-Florence), on April 12-19, 2014, came to the editorial office on 14.03.2014

SIMULATION OF HYDROGEN-AIR PEMFC

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Nowadays it is increasingly important to search new energy systems based on the use of pure and inexhaustible energy sources. Attractiveness of hydrogen as a universal energy is caused by its environmental cleanliness, flexibility and efficiency of energy conversion processes with its participation.

The aim of this work is to simulate the low operating temperature hydrogen-air polymer electrolyte membrane fuel cell (PEMFC) for generation of electricity using as a fuel gas containing impurities of methane and carbon oxide. At creating a PEMFC the main attention is focusing on the development of catalysts with enhanced tolerance to methane and carbon oxide in the fuel.

PEMFC is a complex system, its characteristics are determined by parameters of each component. Developed mathematical model of the PEMFC is based on the basic equations of hydrodynamics, conservation equations of mass, energy and current. The model takes into account the influence of the catalyst layer active area, the platinum content of the catalyst in the active layer, its overall characteristics on the current and the power produced by the FC.

Mathematical model includes the following equation: potential equation, local surface over-potential equations at anode and cathode, the boundary conditions for the potential and equations calculating current density at anode and cathode.

The model treats the following processes: transport of water and reagents in bipolar plate channels, gas diffusion and active layers, membrane; protons transfer in membrane and active layer of the catalyst; electron flow in the active, gas diffusion layers and electrodes collectors. These areas are described separately in the model and are connected with each by boundary conditions.

The main equations of processes in bipolar graphite plates channels at anode and cathode sides are the laws of components mass conservation and the Navier-Stokes equations for the calculation of gas flow movement. The laws of components mass conservation in the diffusion layers are similar to the previous one, with accounting of layers porosity. The laws of components mass conservation in catalyst layers are similar to laws in the diffusion layers, with the addition of reactions. The law of water mass conservation is in the zone of membrane.

The mathematical model has been tested by comparison with a series of experiments for two types of cathode catalysts: commercial catalyst 40 wt.% Pt/C (E-TEK) -0.4 mgPt/cm^2 and synthesized catalyst.

In the result of simulation the dependences of components concentrations and gas concentration distribution along MEA thickness, the current-voltage characteristics are obtained. Aging of electrochemical active surface due to Pt catalyst poisoning has been simulated.

This study is supported by state contract with Russian Foundation for Basic Research (RFBR) № 14-07-00960.

The work is submitted to the International Scientific Conference «MODERN HIGH TECHNOLOGIES», April 25 - May 2, 2014, Israel (Tel Aviv), came to the editorial office on 18.03.2014