THEORETICAL AND EXPERIMENTAL INVESTIGATIONS OF PEM FC CATALYST LAYERS

Baranov I.E.*, Nikolaev I.I., Grigoriev S.A., Beloglazov V.Yu.
Russian Research Center « Kurchatov institute»
Kurchatov square. 1, Moscow, 123182, Russia
* *E-mail: iv3000@mail.ru*

Fuel elements with polymer electrolyte are widely offered as autonomous power sources. On their basis the creation of power- installations for transport applications is possible. Among advantages of such installations are the simplicity of the device, high efficiency.

The productivity of a polymer electrolyte fuel cell (PEFC) is substantially determined by the quality of development of its catalytic layers. The basic task of development of catalytic layers is the creation of optimal structure of a layer. In such a layer the maximum interface between particles of the catalyst and electrolyte should be realized, with a good electronic and ionic conductivity being maintained. It is also necessary to ensure the transport of gaseous reagents through the ramified porous system existing in a catalytic layer. In order to assure a good electronic and ionic conduction the existence of percolating networks of catalyst and electrolyte particles in the catalyst layer is necessary. Thus, in the layer there should be three interpenetrated percolating networks of particles or volumes: network of particles of the catalyst, electrolyte and pores. The necessity of the three different network systems in the layer makes possible the existence of insignificant volume fraction of one or more system, that can result in the loss of percolation in it. All this speaks about the complexity of the task of optimal layer creation and about the necessity of wide use of modeling methods.

As a result of modeling the structure of the catalyst layer we succeeded to establish the existence of two effects essentially influencing the performance of catalytic layers. It is effect of boundary increase in conductivity of the layer due to the contact to a plane of current collector of separate isolated clusters (Fig1).

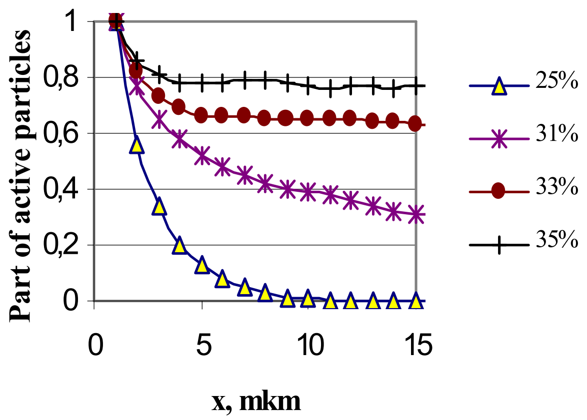

Fig. 1. Distribution of flowing (active) catalyst particles along the layer thickness. Size of catalyst particles 1 μm.

The second effect is the effect of a form of particles in the layer which results in decrease of percolation limit for the particles of essentially elongated forms. (Fig. 2.).

Percolation effects are taken into account in the model of macro kinetic and transport of reactants through porous system of the catalyst layer. Modeling allows to calculate the conditions of flooding of anodic layer by water produced as a result of reaction.

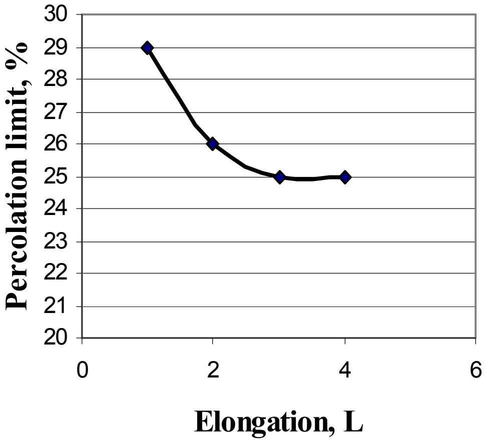

Fig. 2. Dependence of the percolation limit from particle elongation. A particle 3*3*3L

The percolation criterion of the fraction of flooded pours is submitted. It is possible to find the critical size r of pours filled with a liquid from the following condition:

$$\frac{\int_{r}^{\infty} f(r)dr}{\int_{-\infty}^{+\infty} f(r)dr} = 0{,}31$$

Where: f (r) – the distribution function of pours on radiuses; 0,31 – percolation limit. From this equation it is possible to find the diameter above which the pours are filled with liquid and below – with gas.

Experimental researches have shown the influence of the structure and composition of the catalyst layer on its performance. It is shown that at concentration of ionomer close to percolation limit the maximum performance of the layer is observed.

References

1.Baranov. I.E., Fateev V.N., Sysoev A. Modeling of thin catalytic layers with random distribution of particles / // Proceedings of Russian Academia of Science, "Chemistry";–1997; 354(1):55–58.

2. Baranov I.E. et al. Mathematical modeling model of PEM-Fuel Cell catalytic layer. Russian Journal of Electrochemistry 1997; 33(8):967-970.

3. Chirkov Ju.G., Pshenichnikov A.G.// Russian Journal of Electrochemistry 1993; 29(10):1216-1225.