

Numerical optimization of PEM fuel cell electrocatalytic layers via an agglomerate level model

Alexander Kalinnikov, Daria Kriuchkova, and Sergey Grigoriev*

National Research Center “Kurchatov Institute”, 123182 Moscow, Russia

Abstract. The objective of developing the physicochemical model is to formulate recommendations for the fabrication of the membrane–electrode assembly and its components with parameters that meet the requirements imposed on fuel cells. The agglomerate model of the catalytic layers assumes that catalyst particles (platinum on carbon black) are grouped into small spherical agglomerates, each bounded and filled with a polymer electrolyte. Numerical analysis of the cathode catalytic layer shows that the optimal polymer electrolyte content depends on the catalytic layer porosity and air humidity. For porosities in the range of 30–60%, the optimal polymer electrolyte mass fraction lies between 20–30% and decreases with increasing porosity. Increasing air humidity shifts the optimal polymer electrolyte content from approximately 30–40 wt% to about 60 wt%. These results characterize the influence of key parameters on the composition of cathode catalytic layers in proton exchange membrane (PEM) fuel cells. The model-based optimization of cathode catalytic layer structure enhances platinum utilization and minimizes transport losses, enabling reduced noble-metal loading and higher electrochemical efficiency in support of the United Nations (UN) Sustainable Development Goals (SDG 7: Affordable and Clean Energy; SDG 13: Climate Action).

*Corresponding author: sergey.grigoriev@outlook.com

1 Introduction

Large-scale implementation of proton exchange membrane (PEM) fuel cell systems remains constrained by high manufacturing costs and a relatively short service life [1, 2]. These problems are largely related to the constituents of the membrane-electrode assembly (MEA) of fuel cell catalysts based on amorphous carbon black with platinum as the active component (Pt/C) [3]. Catalysts of this composition are expensive and are deactivated under operating conditions due to the dissolution/agglomeration of platinum particles, support corrosion, and detachment of the catalytic layer [4, 5]. Therefore, one of the most important problems in creating fuel cells remains the selection of an effective electrocatalyst carrier that provides low metal loading, high electrochemically active surface area, and high conductivity [6].

In this work, the agglomerate model of catalytic layers was used, which assumes that catalyst particles (platinum on carbon black) are grouped into small spherical agglomerates, bounded and filled with a polymer electrolyte. Electrochemical reactions within the agglomerate are interpreted as reactions in a porous medium. It is assumed that the gas reagent (hydrogen or oxygen) from the gas pores of the catalytic layer dissolves in the electrolyte phase and diffuses through the electrolyte to the reaction centers.

Currently, agglomerate and pseudo-homogeneous models of catalytic layers are used [6, 7], but it is the agglomerate theory that best fits the experimental data. Despite their demonstrated predictive capability, existing based models are often limited in their ability to provide quantitative design guidelines for optimizing catalytic layer composition under realistic operating conditions, particularly with respect to polymer electrolyte content, porosity, and water management. In particular, the combined influence of these parameters on current density distributions and transport losses has not been sufficiently quantified in a form suitable for practical catalyst layer design.

In [8], transport-limited catalyst utilization in polymer electrolyte fuel cell anodes is assessed using an agglomerate model that provides a broader perspective on designing ultra-low Pt-loading, high-performance anodes. The model accounts for electrical- and chemical-potential-driven transport of electrons/protons, and dissolved hydrogen, respectively, as well as multi-component gas-phase transport in the catalyst layer. The model employs the kinetics of the hydrogen oxidation reaction based on a dual-pathway reversible reaction mechanism.

However, the most critical aspect is the consideration of processes in the cathode layer. As part of this work, a physicochemical model was developed, and a numerical analysis of processes in the catalytic layer of a fuel cell was carried out. For specific model calculations, a fuel cell was used containing a membrane, a cathode, an anode catalytic layer, and gas diffusion layers that ideally conduct current and have no diffusion resistance. This model system allows the study of only the catalytic layers.

The purpose of the calculations was to determine the fundamental possibility of operating fuel cells with given electrical parameters. In particular, it may be challenging to achieve an average current density of 1 A/cm² at the voltage of 0.7 V, with air and hydrogen pressures no more than 1.2 bar, and a platinum content no more than 0.1 mg/cm². The task of calculating the catalytic layer was to optimize its composition and water-gas operating regime.

2 Mathematical model

2.1 Agglomerate structure of the cathode catalytic layer

Overall, the catalytic layer comprises a carbon support with catalyst nanoparticles, the surface of which is coated with a polymer electrolyte. The catalyst consists of carbon black particles approximately 30–50 nm in size, on the surface of which nanometer-sized platinum particles are located (Fig. 1). Current generation in the catalyst occurs at the platinum–polymer electrolyte interface. In this case, the protonic current flows through the polymer electrolyte material, while the electronic current flows through the carbon black and platinum particles.

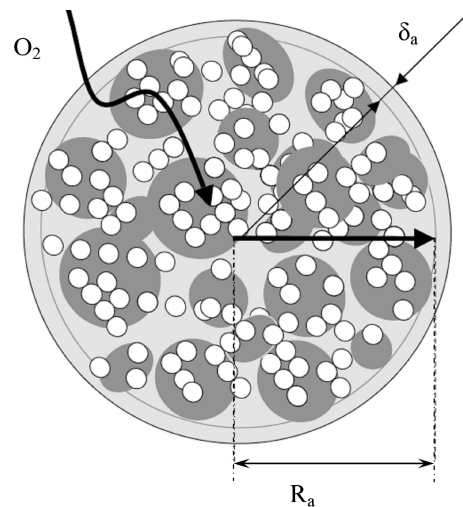


Fig. 1. Agglomerate structure of the cathode catalytic layer.

Oxygen involved in the resulting electrochemical reaction on the surface of the platinum particle diffuses through the polymer electrolyte layer. The product of the resulting electrochemical reaction is water, which is removed from the catalyst through the polymer electrolyte layer. In this case, water removal occurs significantly more efficiently than oxygen supply. This is due to the fact that the effective diffusion coefficient of water in the polymer electrolyte is almost 30 times higher. Therefore, any potential moisture accumulation in the catalytic layer occurs at the interface between the polymer electrolyte, carbon black particles, and catalyst particles.

It is assumed that the catalytic layer is sufficiently thin, and that processes along the interfaces with the membrane and the gas diffusion layer are negligible.

Therefore, all transport equations for the catalytic layers are one-dimensional.

When using the agglomerate model, the following assumptions are made:

- catalytic layer consists of agglomerates containing catalyst particles and ionomer, which are located within the free space (Fig. 1);
- electrochemical reactions occur inside the agglomerates at a constant potential;
- the distribution of catalytically active particles is homogeneous;
- transport of oxygen in the cathode catalytic layer and hydrogen in the anode catalytic layer occurs via dissolution and diffusion of gases in the polymer electrolyte;
- transport of water in the anode and cathode catalytic layer occurs due to capillary forces in the hydrophilic porous medium of the polymer electrolyte.

Similar agglomerates are observed in micrographs of catalytic layers composed of platinum nanoparticles on a carbon support with a polymer electrolyte.

For other fuel cell components, the model has the following limitations:

- diffusion and thermal conductivity processes along the MEA are insignificant in all components except for the bipolar plates, where thermal conductivity in the transverse direction is neglected;
- all transport processes occur at constant pressure. The dependence of the gas phase density on temperature is not taken into account;
- the gases inside the anode and cathode channels are ideal;
- the diffusion medium and catalytic layers are isotropic, and the interfaces with adjacent layers are flat.

2.2 Mass transport

This section presents a mathematical model describing oxygen evolution in the catalytic layer structure under consideration. Below, the electrochemical and mass-transfer processes in the cathode catalytic layer are examined.

The model describes oxygen diffusion in a one-dimensional domain. The region ($0 \leq y \leq \delta_m$) is filled with a polymer electrolyte, within which oxygen diffusion occurs through its porous structure. The equations governing the diffusion processes in this region are given below:

$$\begin{cases} \frac{d^2 P_O^m}{dy^2} = 0 \\ P_O^m(\delta_m) = P_O^{(0)} \\ -D_O^m \frac{1}{RT_{cc}} \frac{dP_O^m}{dy} \Big|_{y=0} = \frac{1}{4F} i_{0c} \left(\frac{P_O^m}{P_O^{ref}} \right) \left(\exp\left(\frac{\alpha_c F}{RT} \eta_{act}\right) - \exp\left(-\frac{\alpha_c F}{RT} \eta_{act}\right) \right) \end{cases} \quad (1)$$

Here:

- D_O^m – diffusion coefficient of oxygen in the polymer electrolyte;
- P_O^m – partial pressure of oxygen in the polymer electrolyte;
- P_O^{ref} – reference oxygen pressure;
- δ_m – thickness of the polymer electrolyte layer;

- α_c – cathodic charge transfer coefficient;
- i_{0c} – cathodic exchange current density;
- R – universal gas constant (8.314 J/mol·K);
- T – absolute temperature;
- F – Faraday constant (96485 C/mol).

Under typical values of the activation overpotential, the second exponential term in the second equation (1) can be neglected. In addition, the following notation can be introduced:

$$\varphi_{tc} = \frac{RT}{\alpha_c F}$$

Where φ_{tc} – cathodic characteristic kinetic potential of the electrode reaction.

The general solution of the formulated problem can be expressed as follows:

$$P_O^m = A_O^m y + B_O^m \quad 0 \leq y \leq \delta_m \quad (2)$$

The unknown constants A_O^m, B_O^m , as well as the oxygen flux, are determined from the boundary conditions. As a result of the transformations, we

obtain:

$$P_O^m = P_O^{(0)} - \frac{\frac{i_0}{P_O^{ref}} \exp\left(\frac{\eta_{act}}{\varphi_{tc}}\right) P_O^0}{\frac{i_0}{P_O^{ref}} \exp\left(\frac{\eta_{act}}{\varphi_{tc}}\right) \delta_m + 4 \frac{\alpha_c}{\varphi_t} D_O^m} (\delta_m - y)$$

(3)

The current is determined by the following

$$\text{relation: } j_c = P_O^{(0)} \frac{\frac{4\alpha_a D_O^m}{\varphi_{tc} \delta_m}}{1 + \frac{4\alpha_c D_O^m P_O^{ref}}{\varphi_{tc} \delta_m i_{0c}} \exp\left(-\frac{\eta_{act}}{\varphi_{tc}}\right)}$$

(4)

Where:

j_c – cathodic current density generated at the surface of an individual catalyst particle;

η_{act} – activation overpotential.

In the limit $\delta_m \rightarrow 0$ (a very thin polymer electrolyte layer) or at high activation overpotential, the maximum current generated by a catalyst particle is obtained and is equal to the maximum rate of oxygen diffusion through the polymer electrolyte layer:

$$j_{maxc} = P_O^{(0)} \frac{4\alpha_c D_O^m}{\varphi_t \delta_m} \quad (5)$$

In this case, the current density generated by a platinum particle is determined solely by the rate of oxygen diffusion through the polymer electrolyte material and does not depend on the value of the activation overpotential. If, under similar conditions, electrochemical reactions occur throughout the entire catalytic layer, mass-transport limitations are observed in the corresponding regions of the current–voltage characteristic (i.e., the current is independent of the output voltage). Under these conditions, the current is also directly proportional to the partial pressure of oxygen.

Using equation (5) for the maximum current j_{max} , the equations for the current density at the surface of the catalytic particle can be rewritten in a form with a clearer physical interpretation. Equation (4) can be transformed as follows:

$$j_c = \frac{J_{\max c}}{1 + \frac{J_{\max c}}{i_{0c}} \frac{P_O^{\text{ref}}}{P_O^{(0)}} \exp\left(-\frac{\eta_{\text{act}}}{\varphi_{\text{tc}}}\right)} \quad (6)$$

At low activation overpotentials, the current is determined by the product of the electrochemical reaction current density and the total surface area of the catalytic particle. This range of activation potentials corresponds to the kinetic regime of the electrocatalytic reaction. When the overpotential is high, current generation is governed by the rate of oxygen diffusion through the polymer electrolyte. In this case, the current density at the catalyst particle reaches its maximum value. It does not increase further, as the activation overpotential continues to grow, becoming limited by oxygen diffusion through the polymer electrolyte phase. The presence of additional diffusion resistance associated with the catalytic layer structure and water accumulation further constrains oxygen transport, thereby limiting the maximum achievable current density. The current density is equal to J_{\max} .

A similar approach to calculating the current in the anode catalytic layer yields analogous equations. The maximum current density is given by:

$$j_{\max a} = P_H^{(0)} \frac{2(\alpha_c + \alpha_a) D_H^m}{\varphi_{\text{ta}} \delta_m} \quad (7)$$

$$\varphi_{\text{ta}} = \frac{RT}{(\alpha_c + \alpha_a)F}$$

The current density in the anode catalytic layer is given by:

$$j_a = \frac{J_{\max a}}{1 + \frac{J_{\max a}}{i_{0a}} \frac{P_H^{\text{ref}}}{P_H^{(0)}} \exp\left(-\frac{\eta_{\text{act}}}{\varphi_{\text{ta}}}\right)} \quad (8)$$

The catalytic layer as a whole provides a specific diffusion resistance to oxygen transport. In addition, the presence of condensed water introduces an additional diffusion resistance to oxygen transport. Taking these factors into account, the equation for J_{\max} should be rewritten as follows:

$$J_{\max} = P_O^{(0)} \frac{4\alpha_c}{\varphi_{\text{tc}}} \left(\frac{D_O}{\delta}\right)_{\text{eff}} \quad (9)$$

Here $\left(\frac{D_O}{\delta}\right)_{\text{eff}}$ – the value of the effective diffusion resistance to transport caused by the factors listed above. This value can be calculated as follows:

$$\left(\frac{D_O}{\delta}\right)_{\text{eff}}^{-1} = \left(\frac{D_O^c}{\delta_c}\right)^{-1} + \left(\frac{D_O^m}{\delta_m}\right)^{-1} + \left(\frac{D_O^w}{\delta_w}\right)^{-1} \quad (10)$$

where $\left(\frac{D_O^c}{\delta_c}\right)^{-1}$ – diffusion resistance of the catalytic layer as a whole; if the generated current is not too high, the electrochemical reactions are localized near the membrane, and the diffusion length δ_c approximately coincides with the thickness of the catalytic layer;

$\left(\frac{D_O^m}{\delta_m}\right)^{-1}$ – diffusion resistance of the polymer electrolyte layer;

$\left(\frac{D_O^w}{\delta_w}\right)^{-1}$ – diffusion resistance of the water layer.

Depending on the parameters of the catalytic layer (porosity, polymer electrolyte content, and thickness), the contributions of the different components of the diffusion resistance vary.

For the anode catalytic layer, the above considerations are analogous. Therefore, the results obtained for the maximum current density in the cathode catalytic layer (9–10) are also applicable to the anode catalytic layer:

$$J_{\max} = P_H^{(0)} \frac{2(\alpha_a + \alpha_c)}{\varphi_{\text{ta}}} \left(\frac{D_H}{\delta}\right)_{\text{eff}} \quad (11)$$

$$\left(\frac{D_H}{\delta}\right)_{\text{eff}}^{-1} = \left(\frac{D_H^c}{\delta_c}\right)^{-1} + \left(\frac{D_H^m}{\delta_m}\right)^{-1} + \left(\frac{D_H^w}{\delta_w}\right)^{-1} \quad (12)$$

The systems of equations (5–12) represent the final solution to the problem considered and define the formulation for the numerical determination of the parameters of the cathode and anode catalytic layers of the fuel cell.

2.3 Charge transport

The total current in the catalytic layers is determined by the sum of the electronic and protonic currents. At the interface between the catalytic layer and the gas diffusion layer, only the electronic current exists, whereas at the interface between the catalytic layer and the membrane, only the protonic current is present. The sum of these currents remains constant throughout the catalytic layer. The mutual conversion of electronic and protonic currents occurs as a result of electrochemical reactions. The formulation of the problem for determining the total current in the cathode catalytic layer is presented as follows:

$$\begin{cases} \frac{d\varphi_{sc}}{dy} = \rho_{sc} J_{sc} \\ \frac{d\varphi_{mc}}{dy} = \rho_{mc} J_{mc} \\ \frac{dJ_{mc}}{dy} = \frac{r_g}{\varphi_{mc} - \varphi_{sc}} x_{cv} (1 - \varepsilon_c) \\ J_{mc} + J_{sc} = J_{0c} \\ J_{sc}(0) = J_0 \quad J_{mc}(0) = 0 \quad \varphi_{sc}(0) = \varphi_{cg}(h_{cg}) \\ J_{sc}(h_{cc}) = 0 \quad J_{mc}(h_{cc}) = J_0 \quad \varphi_{mc}(h_{cc}) = \varphi_m(0) \end{cases} \quad (13)$$

Where:

φ_{sc} – electric potential in the solid (electron-conducting) phase;

ρ_{sc} – effective electrical resistivity of the solid phase;

J_{sc} – electronic current density;

φ_{mc} – electric potential in the proton-conducting phase;

ρ_{mc} – effective ionic resistivity of the polymer electrolyte;

J_{mc} – protonic current density.

In the system of equations (13) $J_c(\varphi)$ – current density generated by a single catalyst particle located at coordinate y within the catalytic layer, as a function of

the activation overpotential. For the cathode catalytic layer, this function is defined by equations (5 – 6).

The overall distribution of current within the catalytic layer can be described as follows. When a load is applied to the fuel cell, current generation begins in the vicinity of the catalytic layer–membrane interface. As the load increases, the current density at the catalytic layer–membrane interface reaches its maximum possible value, after which the region of maximum current generation extends deeper into the catalytic layer.

Water condensation in the catalytic layer begins when the difference between the saturated water vapor concentration and the water vapor concentration in the cathode gas channel is insufficient to provide the mass transport of the required amount of water. In this case, a water film forms within the catalytic layer, creating additional resistance to oxygen diffusion. The process of water condensation in the catalytic layer is governed by mass transport in the gas channel–gas diffusion layer–catalytic layer system.

For the anode catalytic layer, the above considerations are analogous. Therefore, the equations obtained for the current density in the cathode catalytic layer (13) are also applicable to the anode catalytic layer:

$$\left\{ \begin{array}{l} \frac{d\varphi_{sa}}{dy} = \rho_{sa} J_{sa} \\ \frac{d\varphi_{ma}}{dy} = \rho_{ma} J_{ma} \\ \frac{dJ_{ma}}{dy} = \frac{J_a(\varphi_{ma} - \varphi_{sa})}{r_g} X_{av} (1 - \varepsilon_a) \\ J_{ma} + J_{sa} = J_{0a} \\ J_{sa}(0) = J_0 \quad J_{ma}(0) = 0 \quad \varphi_{sa}(0) = \varphi_{ag}(h_{ag}) \\ J_{sa}(h_{ac}) = 0 \quad J_{ma}(h_{ac}) = J_0 \quad \varphi_{ma}(h_{ac}) = \varphi_m(h_m) \end{array} \right. \quad (14)$$

In the system of equations (14) $J_a(\varphi)$ – current density generated by a single catalyst particle located at the coordinate y within the catalytic layer, as a function of the activation overpotential. For the anode catalytic layer, this function is defined by equations (7 – 9).

2.4 Fuel cell parameters used in calculations

The main requirements imposed on the MEA are as follows:

- operating voltage 0.7 V;
- operating current density 1 A/cm²;
- inlet pressure of the reactant gases not exceeding 1.2 bar;
- platinum loading not exceeding 0.1 mg/cm².

The basic components parameters and operating conditions used in calculations are given below.

$\varepsilon_c = \varepsilon_a = 0.35$ – average porosity of the cathode and anode catalytic layers;

$r_s = 3 \cdot 10^{-6}$ cm – average size of carbon black macroparticles (agglomerates);

$x_{cv} = 0.2$ – mass fraction of platinum in the catalyst;

$x_{mv} = 0.25$ – volume fraction of the polymer electrolyte in the catalytic layer;

$h_{cc} = 2 \cdot 10^{-4} / (1 - \varepsilon_c)$ cm – total thickness of the cathode catalytic layer;

$h_{ac} = 7 \cdot 10^{-5} / (1 - \varepsilon_a)$ cm – total thickness of the anode catalytic layer;

$U_{out} = 0.7$ V – output voltage of the model fuel cell;

$X_{wc} = 0.5$ – air humidity;

$X_{wa} = 0.95$ – humidity of the fuel mixture;

$T_0 = 80^\circ\text{C}$ – operating temperature;

$C_H = 0.95$ – hydrogen concentration in the dry fuel mixture;

$m_{Ptc} = 0.1$ mg/cm² – platinum loading in the cathode catalytic layer;

$m_{Pta} = 0.1$ mg/cm² – platinum loading in the anode catalytic layer.

The main parameters of other fuel cell components:

- a parallel bipolar plate channels/ribs arrangement with 1 mm width/height;
- thickness and porosity of anodic and cathodic gas diffusion electrodes are 300 μm and 0.7, respectively;
- proton-exchange membrane thickness 30 μm .

Applicable operating range of the model:

- temperatures between 20 and 80°C;
- voltage 0.3 – 1.0 V;
- current density 0 – 2 A/cm²;
- relative humidity of air and hydrogen 8 – 100%.

The mathematical framework is thoroughly explicated in [9]. The authors developed their own software, utilizing a grid-based approach, to derive the numerical solution for the entire system of equations.

3 Results and discussions

The processes occurring in the cathode catalytic layer are the most critical for the overall performance of the MEA. Therefore, the subsequent analysis is restricted to the cathode catalytic layer. The parameter maps in Fig. 2–3 were obtained by repeating the numerical solution over prescribed ranges of porosity, polymer electrolyte content, and humidity.

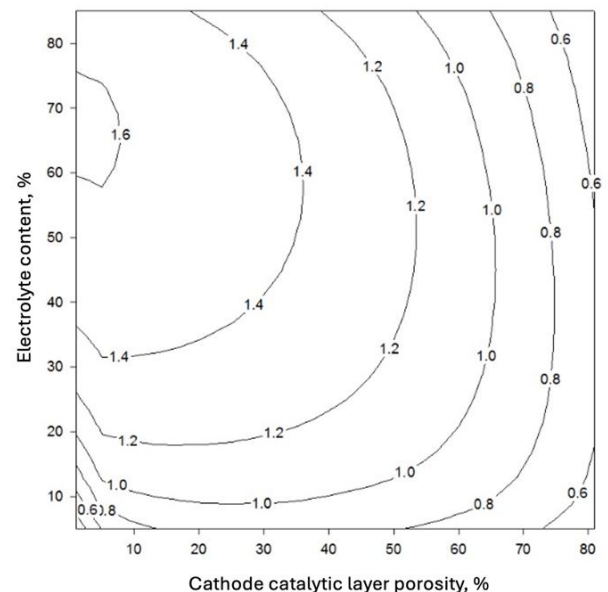


Fig. 2. Lines of equal current density (A/cm^2) in the coordinates of cathode catalytic layer porosity - electrolyte content (wt%).

Analysis of the data in Fig. 2 shows that, for any catalytic layer porosity, there is a polymer electrolyte content that corresponds to a maximum current density. Moreover, the optimal polymer electrolyte content decreases with increasing catalytic layer porosity, and the maximum achievable current density decreases accordingly. At low catalytic layer porosity, the optimal polymer electrolyte content is approximately 60 wt%. At high catalytic layer porosity, the optimal polymer electrolyte content decreases to about 10 wt%.

A low polymer electrolyte content in the catalytic layer results in a high resistance to proton current, while the maximum achievable current density remains high. As a result, the corresponding current-voltage characteristics are expected to exhibit no pronounced mass-transport limitation. At high polymer electrolyte content in the catalytic layer, the layer's ohmic resistance is low; yet, the maximum achievable current is also low. Consequently, in the intermediate current density range, the current-voltage characteristics are expected to be higher. However, at high current densities, the corresponding current-voltage characteristics should exhibit a current limitation due to mass transfer, caused by restricted oxygen diffusion through the polymer electrolyte layer.

Overall, very dense catalytic layers can provide the highest generated currents. In excessively dense layers, a clear tendency toward reduced current is observed due to limitations in oxygen diffusion through the catalytic layer as a whole.

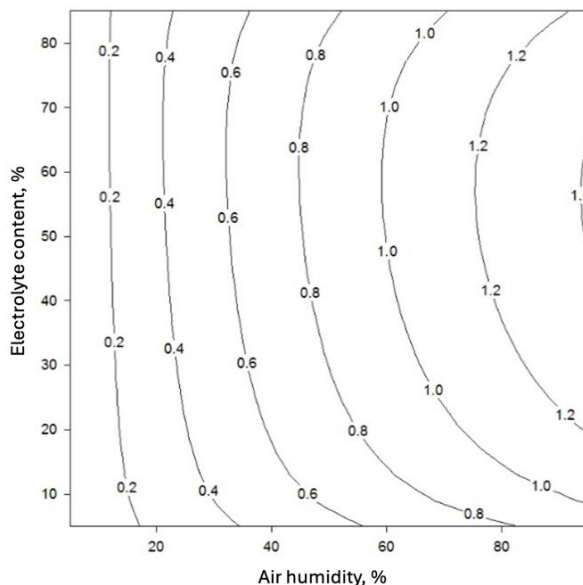


Fig. 3. Lines of equal current density (A/cm^2) in the coordinates of air humidity and electrolyte content.

Analysis of the data presented in Fig. 3 shows that, for any level of air humidity in the catalytic layer, there exists a certain polymer electrolyte content that corresponds to a maximum current density. Moreover, in all cases, increased air humidity leads to higher current density. At low air humidity, the optimal

polymer electrolyte content is approximately 30–40 wt%, whereas at high air humidity it is about 60 wt%.

A low polymer electrolyte content in the catalytic layer, or insufficient humidification, results in a high resistance to proton current and a low resulting current density. At high polymer electrolyte contents in the catalytic layer, the ohmic resistance of the layer is low; yet, the maximum achievable current is also low, which likewise leads to a reduction in the resulting current density.

The highest current density values are achieved at maximum humidification. This is accompanied by flooding of the catalytic layer. The numerical treatment of flooding can only be addressed through calculations for a specific fuel cell channel design. Thus, based on the physicochemical model of the MEA, the composition of the cathode catalytic layer has been optimized.

The calculations performed correlate quite well with the literature data [10-12]. В частности, experimental achieving the targeted performances of 621 mW/cm^2 with cathode Pt loadings 0.12 mg/cm^2 at 80°C , H_2/air and 150 kPa is reported in [11].

4 Conclusions

In this study, the transport-limited catalyst utilization in the polymer electrolyte fuel cell cathode has been numerically analyzed. The simulations were based on an agglomerate structure of the catalyst.

It is shown that the polymer electrolyte content in the cathode catalytic layer at which current generation is most efficient depends on several parameters, including the porosity of the cathode catalytic layer. For catalytic layer porosities of 30–60%, the optimal polymer electrolyte mass fraction lies between 20–30% and decreases with increasing porosity.

In this study, the extent of transport-limited catalyst utilization and its underlying cause are investigated for a conventional cathode catalyst architecture using an agglomerate model, which is simplified but provides the most detailed microstructural description of the catalyst layer. The performance of the engineered catalyst layer designed to overcome both mass and charge transfer limitations is assessed numerically. The results are analyzed to identify the design of an ultra-low Pt loading cathode that exhibits high performance. The numerical calculations have shown the fundamental possibility of operating fuel cells at an average current density more than 1 A/cm^2 and the voltage of 0.7 V , with air and hydrogen pressures no more than 1.2 bar , and a platinum content in electrocatalytic layers of no more than 0.1 mg/cm^2 , highlighting that the identified optimal ranges of polymer electrolyte content and humidification can support lower-Pt cathode designs (UN SDG 7) and improve operational efficiency through reduced transport losses (UN SDG 13).

The work was carried out within the state assignment of NRC “Kurchatov Institute”.

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