The research of compensation for changes in air flow rate by increasing the oxygen concentration of oxidant in a fuel cell

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Abstract. In the article an analytical study of a proton exchange membrane fuel cell (PEMFC) is carried out. The mathematical model describing the electrical properties of the fuel element is given. A distinctive feature of a PEMFC is its increased sensitivity to changes in fuel parameters and a lower one – to changes from outside of the element-oxidant. During operation of the system with a fuel cell a number of accidents, for example caused by a decrease in the rate of the supplied oxidant, is possible. For the simulation of the system operation modes a simulation model in the software environment Matlab/Simulink is developed. Using the model, the possible emergency modes of operation are identified, the possibility of compensation for reducing the rate of the oxidant consumption by increasing the concentration of oxygen in it is investigated. Recommendations for individual and mutual regulation of oxidant parameters and ranges of their concentration are developed.

Keywords – fuel cell, PEMFC, simulation

1. Introduction
In the modern world, a growing trend to switch to cleaner sources of energy is observed. This is resulted from the use of traditional resources which is too dangerous to the planet ecosystem. Besides, traditional energy resources are non-renewable, and, according to forecasts, will run out in the nearest future. Therefore, more attention is paid to the development of alternative and renewable energy and to increasing the generation from these sources. One of the promising alternative energy areas are hydrogen fuel cells. Fuel cells (FC) are environmentally friendly and inexhaustible primary resources, as hydrogen is one of the most common elements on the Earth. The study of the FC modes is important, because the method of generating energy using FC has been only recently applied [1 - 2] and is not investigated in full [3 – 4].

Development of mathematical model and simulation are among the main methods of research, along with the full-scale experiment [5 – 7].

2. Problem Statement
Improvement of electrical properties of alternative sources of energy PEMFC requires a detailed study and analysis of its operation modes. With this purpose it is necessary to determine the influence of PEMFC input parameters on its output characteristics, in particular, to identify the adjustment ranges of the fuel element parameters to determine the sustainable and emergency operation.

3. Theory
A fuel cell is an energy source that produces it in the course of a chemical reaction. The process of chemical reactions occurs on porous electrodes. The atoms of the fuel (hydrogen or hydrogen-
containing substance) supplied to the anode are divided into protons and electrons. Electrons move through the external circuit to the cathode, creating direct electric current. Protons move to the cathode through electrolyte. At the cathode reduction reaction occurs, protons and electrons are combined with the oxidant (oxygen or air) to form water. The products of this reaction are heat and water vapor.

The figure shows a schematic diagram of the FC proton exchange membrane [3].

![Schematic diagram of fuel cell proton exchange membrane](image)

**Figure 1.** Schematic diagram of fuel cell proton exchange membrane

Reactions occurring in the cell can be described by the following expressions:

On the anode:

\[ \text{H}_2 \rightarrow 2\text{H}^+ + 2e^- ; \]

On the cathode:

\[ \frac{1}{2}\text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} ; \]

The overall reaction in PEMFC:

\[ \text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O}. \]

4. **FC mathematical model**

Using a detailed model of a fuel cell, it becomes possible to study changes of its input parameters, such as pressure, temperature, concentration and flow rates of fuel and oxidant. Changes in these parameters affect the open-circuit voltage \(E_{OC}\), the exchange current \(i_0\) and the Tafel slope \(A\). \(E_{OC}\), \(i_0\) and \(A\) are modified as follows:

\[ E_{OC} = K_cE_n \]  \hspace{1cm} (4)

\[ i_0 = \frac{zFk(P_{H2}+P_{O2})}{R_h} e^{\frac{-\Delta G}{RT}} \]  \hspace{1cm} (5)

\[ A = \frac{RT}{zF} \]  \hspace{1cm} (6)
where R = 8.3145 j/(mol K); F = 96485 AV/mol, z = the number of moving electrons, En = the Nernst voltage, which is the thermodynamics voltage of the cells and depends on the temperature and partial pressure of reactants and products inside the stack (V); α = the coefficient of charge transfer, which depends on the type of electrodes and catalysts; \( P_{\text{H2}} \) is the partial pressure of hydrogen inside the stack (ATM); \( P_{\text{O2}} \) is the partial pressure of oxygen inside the stack (ATM); K = is the Boltzmann constant is equal to \( 1.38 \times 10^{-23} \)J/K; h = is the Planck constant = \( 6.626 \times 10^{-34} \) J s; \( \Delta G \) = is the size of the activation barrier which depends on the type of electrode and the catalyst used, T = is the operation temperature (K); KS = is a constant voltage at the nominal operating conditions.

The rate of conversion (use) of hydrogen (\( U_{\text{H2}} \)) and oxygen (\( U_{\text{O2}} \)) are determined in the following way:

\[
\begin{align*}
U_{\text{H2}} &= \frac{n_{\text{H2}}}{n_{\text{H2}}^\text{nom}} = \frac{60000RT_{\text{fuel}}}{2FP_{\text{fuel}}V_{\text{tpm(fuel)}}x}\% \\
U_{\text{O2}} &= \frac{n_{\text{O2}}}{n_{\text{O2}}^\text{nom}} = \frac{60000RT_{\text{fuel}}}{2FP_{\text{air}}V_{\text{tpm(air)}}y}\%
\end{align*}
\]  

(7)  

(8)

where \( P_{\text{fuel}} \) = is the absolute fuel supply pressure (ATM); \( P_{\text{air}} \) = is the absolute air supply pressure (ATM); \( V_{\text{tpm(fuel)}} \) = is the fuel consumption (l/min); \( V_{\text{tpm(air)}} \) = is the air flow (l/min); \( x \) = is the percentage of hydrogen in the fuel (%); \( y \) = is the percentage of oxygen in the oxidant (%); \( N \) = is the number of cells.

Constant 60000 comes from the conversion from flow speed l / min used in the model, to the dimensionality of m³/s (1 liter / min = 1/60000 m³/sec).

Partial pressure and the Nernst voltage are determined as follows:

\[
\begin{align*}
P_{\text{H2}} &= \left(1 - U_{\text{H2}}\right)x\%P_{\text{fuel}} \\
P_{\text{H2O}} &= \left(w + 2yU_{\text{O2}}\right)P_{\text{air}} \\
P_{\text{O2}} &= \left(1 - U_{\text{O2}}\right)y\%P_{\text{air}}
\end{align*}
\]  

(9)  

(10)  

(11)

\[
E_{\text{nernst}} = \begin{cases} 
1.229 + (T - 298)\frac{-44.43}{xF} + \frac{RT}{2F}ln\left(\frac{P_{\text{H2}}p_{\text{O2}}^{1/2}}{P_{\text{H2O}}}\right) & \text{при } T \leq 100^\circ \text{C} \\
1.229 + (T - 298)\frac{-44.43}{xF} + \frac{RT}{2F}ln\left(\frac{P_{\text{H2}}p_{\text{O2}}^{1/2}}{P_{\text{H2O}}}\right) & \text{при } T > 100^\circ \text{C}
\end{cases}
\]

(12)

where \( P_{\text{H2O}} \) = is the partial pressure of water vapor inside the stack (ATM); \( W \) = is the percentage of water vapor in the oxidant (%).

From the partial gases pressures and the Nernst voltage the new values of open circuit voltage (\( E_{\text{OC}} \)), the exchange current (\( i_0 \)) and the Tafel slope (A) can be calculated.

The parameters \( \alpha, \Delta G \) and \( Kc \) are calculated based on the polarization curve at nominal conditions of operation along with some additional parameters, such as the low efficiency of the calorific value of the stack, composition of fuel and air, gas pressure and temperature. They can be easily taken from the manufacturer specifications.

Nominal levels of gases conversion are calculated as follows:

\[
U_{\text{H2}} = \frac{\eta_{\text{nom}}\Delta h^b(H_2O(gas))N}{2FP_{\text{fuel}}V_{\text{tpm(fuel)}}}\]

(13)

\[
U_{\text{O2}} = \frac{60000RT_{\text{fuel}}\eta_{\text{nom}}}{2FP_{\text{air}}V_{\text{tpm(air)}}y_{\text{nom}}0.21}
\]

(14)
where $\eta_{\text{nom}}$ – is the nominal stack efficiency of STC (%), $\Delta h^d$ (H2O (gas)) – 241.83 × 103 j/mol; $V_{\text{nom}}$ – is the nominal voltage (V); $I_{\text{nom}}$ – is the nominal current (A); $V_{\text{lpm(air)nom}}$ – is the nominal air flow (l/min); $P_{\text{airnom}}$ – is the rated absolute supply pressure of air (PA); $T_{\text{nom}}$ – is the nominal operating temperature (K).

The nominal partial pressure of gases and the Nernst voltage can be obtained from the conversion rate. If $E_{\text{OC}}$, $i_0$ and $A$ are specified and if it can be assumed that the stack operates at a constant rate of conversion or is used under nominal conditions, then $\alpha$, $\Delta G$ and $K_C$ can be determined.

5. Simulation

For simulation of fuel cell at constant load and study its performance response to key parameters changes, a simulation quantitative model in software environment MATLAB/Simulink was developed.

The assembled model is shown in figure 2.

**Figure 2. Simulation model of the fuel cell**

The nominal voltage of the fuel cell 45 V dc is applied to the voltage converter. The transformer increases the voltage to 100 V dc, then the voltage is applied to a constant load, with interval time of 1 sec. The nominal power of the unit is 6 kW.

6. Experimental results

A distinctive feature of proton exchange membrane fuel cells is their increased sensitivity to changes in fuel parameters and a lower one – to changes from outside of the element-oxidant. Although the change of the oxidant parameters is less critical, it can have a significant impact on the FC functioning and its output characteristics. For this simulation model the nominal values of the oxidant are the following: the oxygen content in the oxidant is at the level of 21 % (normal air), the air flow rate is 300 l/min.

During operation of the system with fuel cell as a power supply, some emergency situations can occur. The reason for operating emergency conditions can be a decrease in the rate of the supplied oxidant. For proper functioning of the fuel cell and the normal flow of chemical reactions, a certain amount of oxidant is necessary.

To avoid FC emergency operation mode, the effect of reducing the air flow rate must be compensated by changes in another parameter. This parameter can be the percentage of oxygen in the oxidant. To study the feasibility of this type of compensation two introductory signals modified at the same time were specified. The first signal (figure 3) is responsible for reducing the air flow rate from...
300 l/min to 200 l/min. The second input signal (figure 4) is responsible for the change of the oxygen concentration in the oxidant.

![Figure 3](image1.png)

**Figure 3.** Input responsible for reducing the air flow rate

![Figure 4](image2.png)

**Figure 4.** Input responsible for the increase in the oxygen concentration in the oxidant

Up to the tenth second there is the start in the fuel cell, and all the input parameters take the nominal values. Starting with second 10, occurs the ramp change of: the air flow rate is reduced from 300 l/min to 200 l/min, oxygen concentration in the oxidant increases from 21% to 2.5%. The value of 2.5% is the minimum increase in the oxidant concentration in such a significant reduction in the rate of its consumption. Changes in the concentration of oxygen in a smaller range prevents normal operation of the fuel cell by reducing the air flow rate.

During the simulation of the air flow rate reduced compensation by increasing the concentration of oxidant by 2.5%, graphs of the fuel cell output current and voltage are shown in figures 5 – 6.
7. Results and discussion

For the normal operations of the fuel cell, nominal values for all input parameters should be kept including the air flow rate, since at a low value of this parameter the oxidant will not be sufficient for the reaction. As it was found during the simulation, in the studied simulation model the air flow rate reduction up to 200 l/min can be compensated by increasing the oxygen percentage of the oxidant by only 2.5%.

We can safely adjust these two parameters in two ways:
- simultaneously;
- first, to increase the concentration of oxygen in the oxidant, then, to reduce the consumption of oxidant.

Initially, it is impossible to safely reduce the consumption of the oxidant with a subsequent increase in the oxygen concentration. This will lead to an emergency operation mode of the fuel cell and the current increase up to several kilo-ampers.
8. Conclusion

- The FC simulation model is developed.
- The possibility of compensation for reducing the rate of oxidant consumption, by increasing the oxygen concentration in it is studied.
- It is revealed that the decrease in the rate of air flow by 100 l/min can be compensated by an increase in the oxygen concentration in the oxidant by 2.5% rather than to exclude the FC emergency mode. Regulation recommendations by using this method are developed.

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