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COMPUTATIONAL ANALYSIS OF PEM FUEL CELL UNDER DIFFERENT OPERATING CONDITIONS

Abstract

PEM fuel cells are one of the most promising sources of electrical energy and also have interesting properties. This research is purely theoretical and based on ANSYS Fluent software. Thus, the next step of the research should be the comparison of the solutions to other models and experimental results. The PEM fuel cell can be used as an energy source in the near future in a much more common way, although there are few modifications required, such as increasing efficiency and reducing production costs.
In general, a three-dimensional steady-state model of the polymer electrolyte membrane fuel cell implemented in Fluent was used to study a single channel flow inside such a PEMFC. The analysis concerns an aspect, that seems to be overlooked in this type of analysis, namely the influence of the substrate flow rate on the quality and efficiency of the chemical reaction, and thus on the value of the generated current for a given voltage. It is clearly visible that there is a rather narrow range in the amount of hydrogen fuel fed that is optimal for a given fuel cell. Such theoretical research is very useful and very much needed to design a new PEM fuel cells, utilizing Computational Fluid Dynamics (CFD) tool to statically monitor its performance for different boundary conditions.

1. INTRODUCTION

Fuel cells are a promising technology for generating electricity with high efficiency and low environmental impact. They belong to the category of unconventional energy sources, that is, those which are not based on traditional fossil fuels such as coal, oil, or natural gas. Instead, they utilize renewable or alternative sources of energy such as wind, solar, geothermal and hydrogen, that do not generate carbon dioxide pollution (Khalil, 2018).

Hydrogen fuel cells find many applications in various industries. First of all, they can be found in power industry by supplying energy to places where it is impossible to ensure free access to the power grid. Secondly, they apply in automotive on an ever-increasing scale. Other applications of such a technology are as follows: construction of autonomous robots, alarm power systems, space technologies - ships and probes and many more. Over the last few years, more and more large institutions or entire housing estates have been investing in hydrogen technology for powering and heating apartments or houses. In Poland, for

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example, it is a housing estate in Środa Śląska or an investment in the commune of Śrem. Of course, pioneering ideas in other countries already work and pass the exam.

The use of hydrogen cells in the automotive industry is especially worth paying attention to. Hydrogen cell engines are a solution that is used by an increasing number of car manufacturers. There are already several models from top brands with such a drive - the efficiency of hydrogen fuel cells is quite high, which allows them to be used even in buses and trucks. Summing up, research in the field of high-energy hydrogen power systems is developing all over the world and is one of several groundbreaking and heavily invested technologies such as quantum engineering or space technologies.

Conventional power plants convert chemical energy into electrical energy in three steps: production of heat by burning fuel, conversion of heat into mechanical energy (here the efficiency is limited by the Second Law of Thermodynamics) and finally conversion of mechanical energy into electrical energy. Thus, the efficiency of such a process is low. Fuel cells are a type of energy technology that converts the chemical energy of a fuel directly into electrical energy without combustion, where two half-reactions occur at the electrodes. On anodes fuel is oxidised and on cathodes oxygen is reduced. Polymer electrolyte membrane (PEM) fuel cells belong to a type of fuel cells that use hydrogen as the fuel and oxygen as the oxidant to generate electricity. The electrochemical reaction between hydrogen and oxygen produces water, heat, and electricity. This renders them an exceptionally clean and environmentally friendly method of energy production. They can work at relatively low temperatures compared to traditional combustion technologies (Askaripour, 2019).

Its catalytic properties cause the hydrogen molecule to break down into H^+ ions and electrons, where platinum is used as a catalyst usually. In PEM fuel cells, the membrane, as the electrolyte, is applied and it is typically made of a polymer material that is highly conductive to protons. While protons move through the electrolyte, electrons are transported through an external circuit to the cathode. More information about this technology can be find in work (Albarbar & Alrweq, 2018).

There are still some challenges, when it comes to the commercialization of PEM fuel cells, such as the high cost of the technology and the limited availability of hydrogen fueling infrastructure (Tellez-Cruz et al., 2021). This work is devoted to the analysis of the effect of hydrogen feed rate on the amount of generated current. The thesis examines how changing the hydrogen delivery rate affects the performance of a fuel cell. Such analyses are taken very often in different works (Qin et al., 2022; Yue-Tzu et al., 2012; Ahmadi & Rostami, 2019; Haddad et al., 2015; Zeroual et al., 2012). The results of the study are expected to provide valuable insights into the optimization of PEM fuel cells for various applications (Hinaje et al., 2012).

2. FUEL CELL MODEL

The analysis of the phenomenon in the CFD software consists of three basic parts: the first - preprocessing, which involves building a geometric model and then discretizing it into finite elements, the second - solving the problem, which involves numerical solving of fundamental equations and optionally other equations describing selected models of phenomena, for each finite element, which determines the parameters of interest, the third - postprocessing, i.e. the last stage in which the test results are visualized.

Ansys was founded in the United States in 1970. It is currently the largest producer of design, analysis and simulation software. It allows one to perform complex engineering calculations and offers many extensions that enrich the application, such as Fluent, which is an execution-enabled environment. It uses an intuitive interface that allows for any interaction with the model during the design and calculation process. In the world, almost 4000 companies, including very large ones, use this software as their basic development activity, not to mention scientific institutions, of which there are also a large number.

Below, in Fig. 1, there is a graphic showing the user interface of Fluent software in version 2022 R2, which shows the possibilities offered by this software, detailing the methods of solving equations describing the phenomena occurring in the fuel cell selected in this work and the residuals on the right.

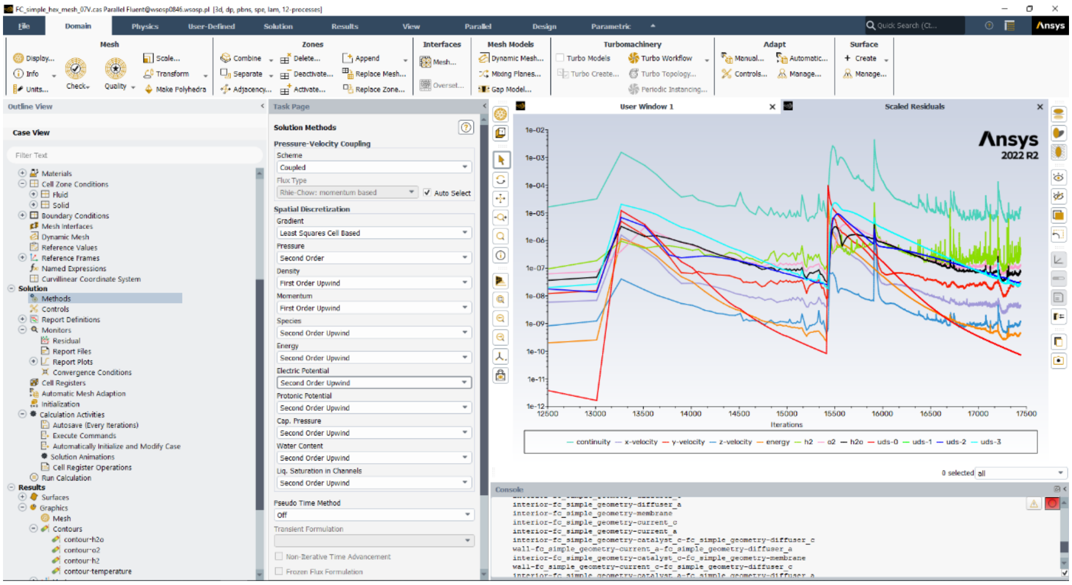

Fig. 1. Fluent interface

2.1. Geometric model

To begin considerations on the impact of the amount of fuel fed on the generated current in the fuel cell, based on the CFD method, a model of the fuel cell was designed using the ANSYS SpaceClaim software, shown in Fig. 2. It consists of elements of a classic PEMFC, such as: current collectors, flow channels, porous electrodes, catalyst layers as well as the membrane. Electrical tabs were named 'voltage_a' and 'voltage_c'. The geometry also includes 'inlet_a', 'inlet_c' as well as 'outlet_a' and 'outlet_c'. The symbol 'a' stand for the anode and 'c' for the cathode. In addition, two areas of contact resistivity have been introduced between flow channels and porous electrodes with 2.10-6 ohms/m2 resistivity.

Tab. 1. Geometric parameters in PEMFC model

Quantity	Value
Gas channel depth	1 mm
Gas channel width	1 mm
Gas channel length	10 mm
Gas diffusion layer thickness	0.025 mm
Catalyst thickness	0.01 mm
Membrane thickness	0.03 mm

With the domain determined in this way, meshing was performed using the ANSYS Meshing software. The computational mesh was made based on hexahedral elements, due to very simple geometry model. The total number of elements is 893000 with a minimum orthogonality of 0.6169546. According to the paper (Zhang et al., 2021), where the dependence of the results on the mesh density was examined for a full fuel cell, not only for one channel, it is indicated that the number of 707556 mesh elements is sufficient. In this work, 893000 elements were obtained for only one channel. The whole obtained mesh is presented in Fig. 3, while its details are shown in a close-up in Fig. 4. Blue arrows indicate inlets to the channels.

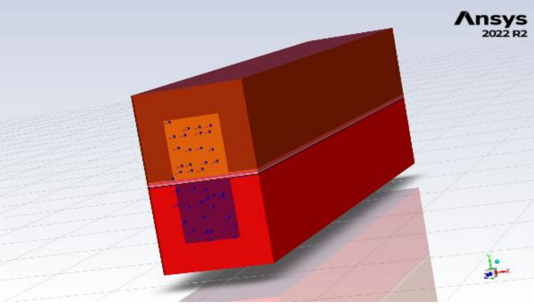

Fig. 2. PEMFC geometry

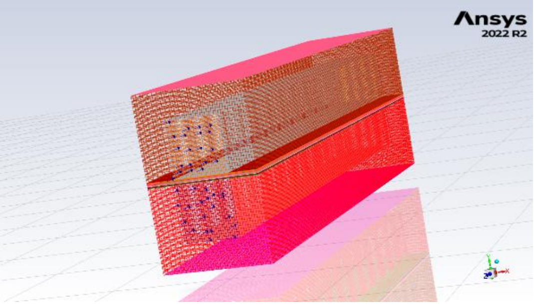

Fig. 3. PEMFC mesh

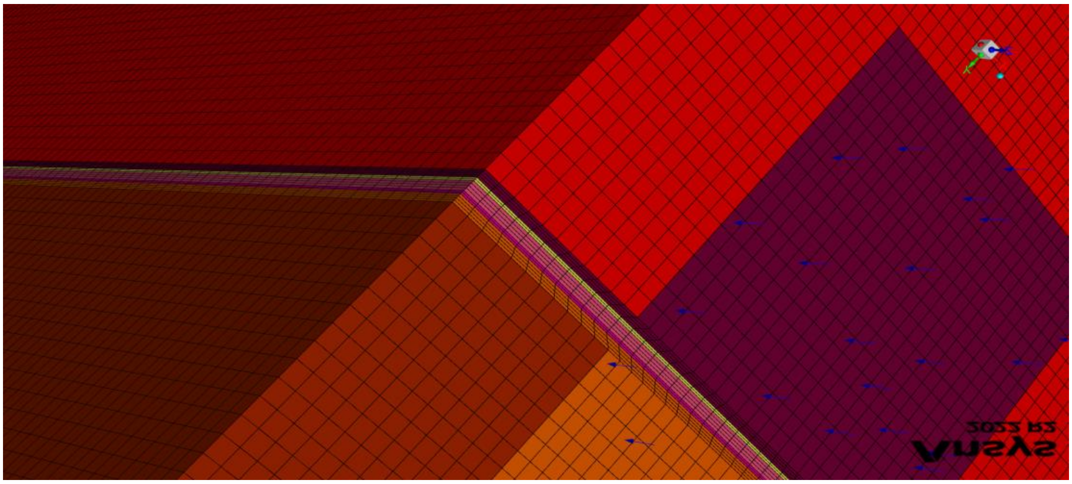

Fig. 4. PEMFC mesh details

2.2. Mathematical model

The mathematical model adopted in the work is a 3D model implemented in ANSYS Fluent software as an PEMFC add-on module. Of course, there are also other possible models adopted to study behavior of PEMFC for different conditions in both 1D and 3D (Falcão et al., 2011; Akhtar & Kerkhof, 2011) to choose. Equations used during our numerical solutions are listed in Tab. 1. The authors recommend, that interested persons familiarize themselves with the explicit forms of the equations adopted in the mathematical model presented and well explained in (ANSYS Fluent Theory Guide, 2022). The most important governing equations are as follows, where related symbols can be referred to in (ANSYS Fluent Theory Guide, 2022):
mass conservation equation:

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla(\varepsilon\rho\vec{u}) = S_m\ , \tag{1}$$

momentum conservation equation:

$$\frac{\partial(\varepsilon\rho\vec{u})}{\partial t} + \nabla(\varepsilon\rho\vec{u}u) = -\varepsilon\nabla p + \nabla(\varepsilon\mu\nabla\vec{u}) + S_u\ , \tag{2}$$

energy conservation equation:

$$\frac{\partial(\varepsilon\rho c_p T)}{\partial t} + \nabla\left(\varepsilon\rho c_p\vec{u}T\right) = \nabla\cdot(k^{eff}\nabla T) + S_Q\ , \tag{3}$$

species conservation equation:

$$\frac{\partial(\varepsilon c_k)}{\partial t} + \nabla(\varepsilon\vec{u}c_k) = \nabla\cdot(D_k^{eff}\nabla c_k) + S_k\ . \tag{4}$$

Tab. 1. Equations included in PEMFC mathematical model

Equations	Logic value
Flow	True
h2	True
o2	True
h2o	True
Energy	True
Electric Potential	True
Protonic Potential	True
Cap. Pressure	True
Water Content	True

Assumptions used in the fuel cell modeling are:
- ideal gas properties,
- laminar flow,
- isotropic and homogeneous electrolyte, electrode, and bipolar material structures,
- a negligible ohmic potential drop in components,

- mass and energy transport is modeled from a macroperspective using volume-averaged conservation equations,
- a porous area including membrane, catalyst layers and gas diffusion layers are considered to be isotropic.

The solver was chosen as pressure-based and steady-state in double-precision mode. All solution methods are presented in Tab. 2. The Warped-Face Gradient Correction was added to solutions.

Tab. 2. Solution methods

Pressure-velocity coupling	**Coupled**
Spatial discretization for	
Gradient	Least squares cell based
Pressure	Second order
Density	First order upwind
Momentum	First order upwind
Species	Second order upwind
Energy	Second order upwind
Electric potential	Second order upwind
Protonic potential	Second order upwind
Cap. pressure	Second order upwind
Water content	Second order upwind

According to calculated Reynolds number, flows inside fuel cells are laminar and no turbulence model is included in equations used in this work finally. On the other hand, turbulent flows are characterized by rapid processes that are very helpful in mixing the layers and thus facilitate better reaction between atoms, which should contribute to improving the properties of fuel cells as a whole. According to the authors, this type of research should be conducted both at the theoretical and experimental level.

2.3. Boundary and operating conditions

For such a selected set of equations, describing the physics of the processes occurring in the designed geometry of the fuel cell, constants of the model and boundary conditions should be assumed. As for most of the constants contained in the mathematical equations, they have remained unchanged and have default values adopted in Fluent. The values of these constants can be checked in (ANSYS Fluent User's Guide, 2022).

For solutions, the ideal gas with Clapeyron equation was assumed for all gasses. As far as boundary conditions for inlets are considered 'mass-flow-inlet' was chosen and 'pressure-outlet' for outlets. On external contact boundaries, the values of potential are fixed as potential static boundary conditions. In this model, the potential on the anode side is set as 0 and on the cathode side as 0.75 V.

Tab. 3. Operating conditions

Parameters	Values
Working temperature	333 K
Operating pressure	150000 Pa
Open circuit voltage	0.75 V
Gravity	No
Mass flow for anode (0.6 – h2, 0.4 – h2o)	from $8 \cdot 10^{-10}$ to $9 \cdot 10^{-7}$ kg/s
Mass flow for cathode (0.15 – h2o, 0.21 – o2)	10^{-6} kg/s

3. RESULTS AND DISCUSSIONS

In order to verify the correctness of the results obtained in this theoretical work, in Fig. 5 a comparison of both CFD and experimental polarization curves for PEMFC was shown. These experimental curves comes from work (Zhang et al., 2009) and are obtained for very similar cell operating parameters. The pressure assumed during our calculations is 1.5 atm and a comparison is presented for the curves obtained for similar fuel cell operating pressures, i.e. for the pressure of 1 and 2.02 atm. It can be seen that for the most part, the curves coincide quite well, except for the areas with low voltage and high currents. This is an issue that needs to be explored in more detail in future work. From the picture can be noticed, that the greatest inaccuracy of the results obtained in this work compared to the experimental results is for the voltage value about 0.8 V, where the percentage error is about 10 compared to 1 atm pressure received in the experiment.

Having such a justified correctness of the solution, the analysis of the dependence of the generated current on the hydrogen supplied to the anode was started. The results are presented and discussed below.

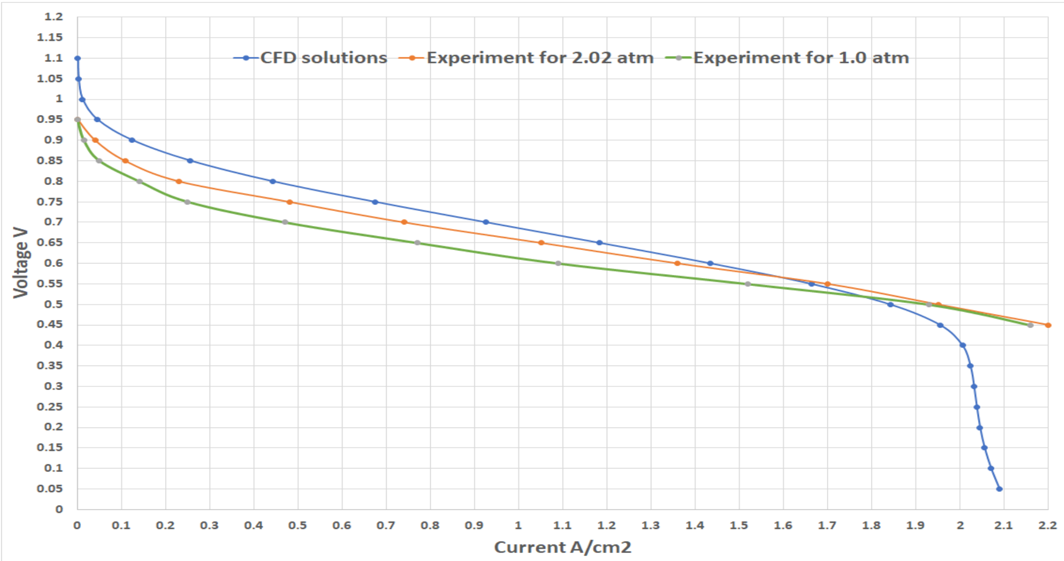

Fig. 5. Polarization curves: blue line – CFD solutions for 10^{-7} kg/s mass flow rate, red line – experiment for 2.02 atm pressure, green line – experiment for 1.0 atm pressure (Zhang et al., 2009)

As already mentioned, one of the problems related to the commercialization of fuel cells is the availability of pure hydrogen. Due to the limited resources these days of this fuel, proper hydrogen supply is important. The analysis showed, that there is a clear limit, where further increasing the mass flow of supplied hydrogen does not increase the current obtained for a given voltage and a given air mass flux. On the other hand, after exceeding a certain minimum mass flux of hydrogen, the amount of current generated by the cell drops quite sharply, having constant the remaining parameters of the fuel cell. It is significant that, what can be seen form Fig. 6, increasing the amount of hydrogen almost does not change the current generated by the analyzed fragment of the PEM fuel cell starting from about 0.3 μg/s. It can also be read from Figure 6 that for a mass flow rate of less than 0.1 μg/s, the current begins to drop quite rapidly. To show this region more precisely, the currents for mass flow rates ranging from 0.008 to 0.1 μg/s are shown in the next Fig. 7.

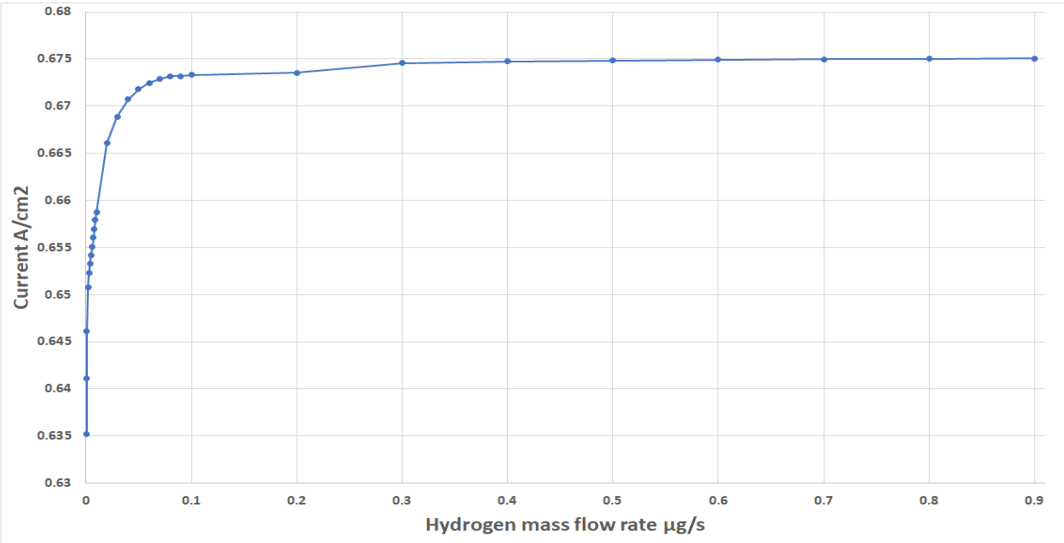

Fig. 6. Dependence of the generated current on the hydrogen mass flux for the whole range of analyses

Looking at the diagram shown in Fig. 7 it can be seen that from $8 \cdot 10^{-2}$ to $2 \cdot 10^{-2}$ μg/s of hydrogen flux, the current starts to decrease quite slightly from 0.673 A/cm^2 value to 0.666 A/cm^2. Further reduction of the hydrogen mass flux results in a very marked decrease in the current. From $2 \cdot 10^{-2}$ μg/s to $3 \cdot 10^{-3}$ or even $2 \cdot 10^{-3}$ μg/s the current is linearly reduced to 0.651 A/cm^2. And finally, from that point on, the current drop is rapid. Summing up these considerations it can be indicated, that for the analyzed case the best mass flux value should be in the range from 0.01 to 0.1 μg/s.

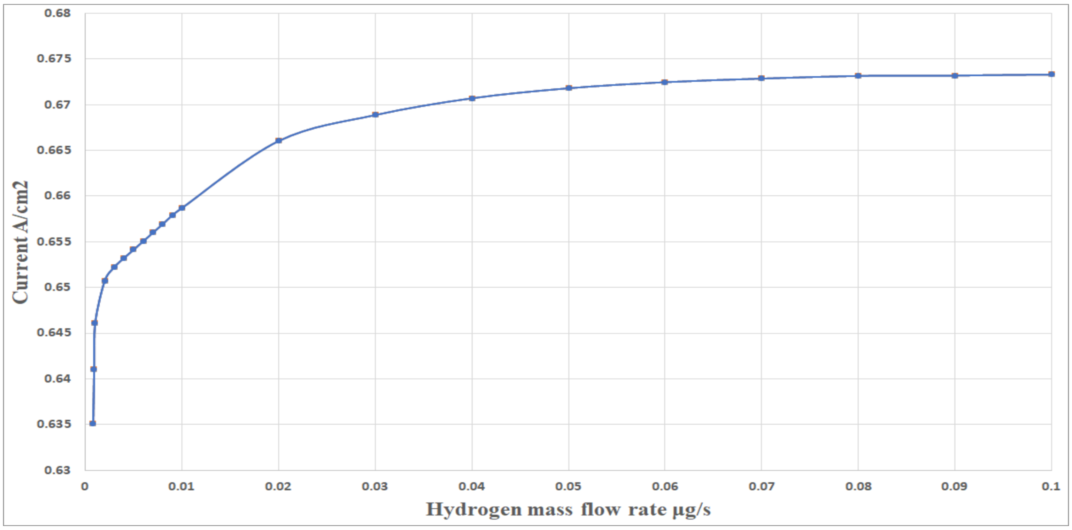

Fig. 7. Dependence of the generated current on the hydrogen mass flux for the range from 0.0008 to 0.1

In order to visualize the mass distribution of hydrogen in the anode channel in more detail, the following figures show the mass fraction of hydrogen on the symmetrical cross-section of the anode and cathode channels. The blue color indicates zero hydrogen content in the cathode channel. The change of hydrogen distribution, including the drop of the pressure in the fuel cell, was analyzed in work (Pei et al., 2006) to compare.

From the boundary conditions it is known that the mass fraction in the inlet was 0.6 for hydrogen. It is very clear that for the value of 0.6 µg/s, according to Fig. 8, the vast majority of hydrogen supplied to the channel flows out of it, without reacting with oxygen, generating very large fuel losses. In order to obtain a stoichiometric composition, it is necessary to carefully analyze the proportions of the supplied hydrogen fuel and oxygen or air.

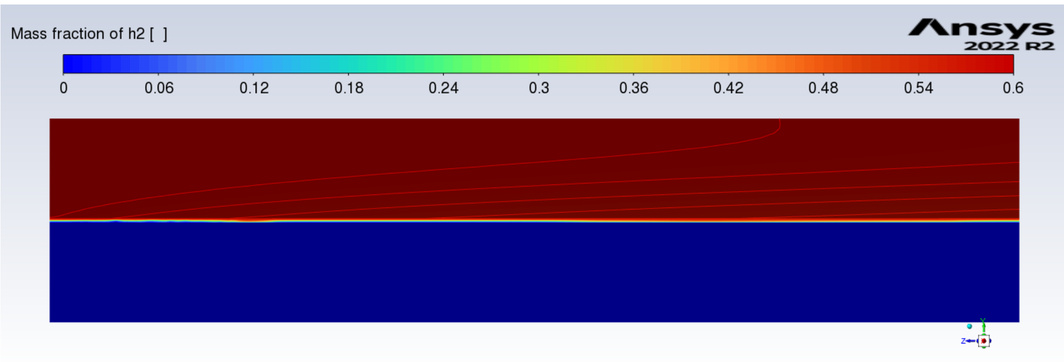

Fig. 8. Mass fraction of h2 on the plane of symmetry at the cathode and anode for 0.6 µg/s

In turn, Fig. 9 shows the mass fraction of hydrogen for the mass flow rate on the inlet equal to 0.06 µg/s, which is 10 times smaller compared to the previous figure. Here we have a pronounced decrease in the hydrogen content, but also it is clear, that in this case huge losses of hydrogen fuel are generated. At the end of the channel, a decrease from 0.6 to about

0.5 mass fraction of hydrogen can be seen. Let us remember that for a mass flow rate of 0.6 μg/s the current value is 0.675 A/cm2 and for a tenfold decrease in the amount of hydrogen we have a decrease in current only to the value of 0.6725 A/cm^2.

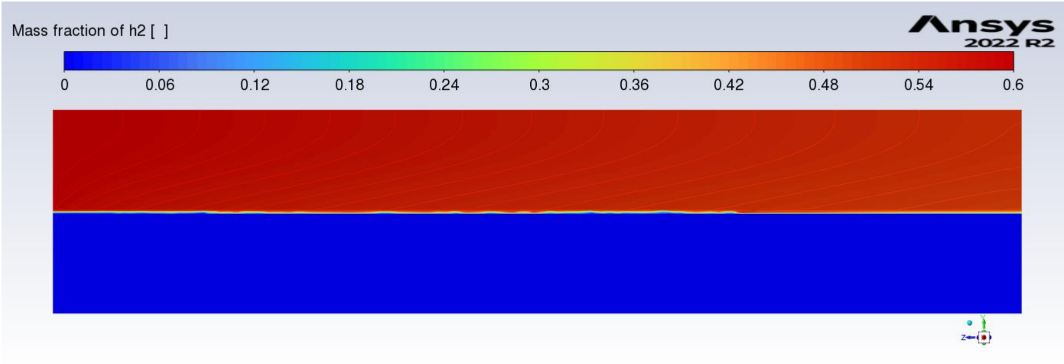

Fig. 9. Mass fraction of h2 on the plane of symmetry at the cathode and anode for 0.06 μg/s

The next Fig. 10 shows the mass flow rate of 0.006 μg/s, which is 100 times lower than in Fig. 7 and 10 times lower than in Fig. 8. In this case, we already have a quite clear decrease in the amount of hydrogen in the channel that has been reacted, but in this case it is also not a favorable proportion of hydrogen in relation to the supplied air. From a value of 0.6 at the inlet of the channel, the amount of hydrogen decreased to a value of approximately 0.4 at the end. In addition, for such a mass flow rate, the current obtained is also high and amounts to 0.655 A/cm^2. This is still a very slight drop in current comparing to hydrogen saved.

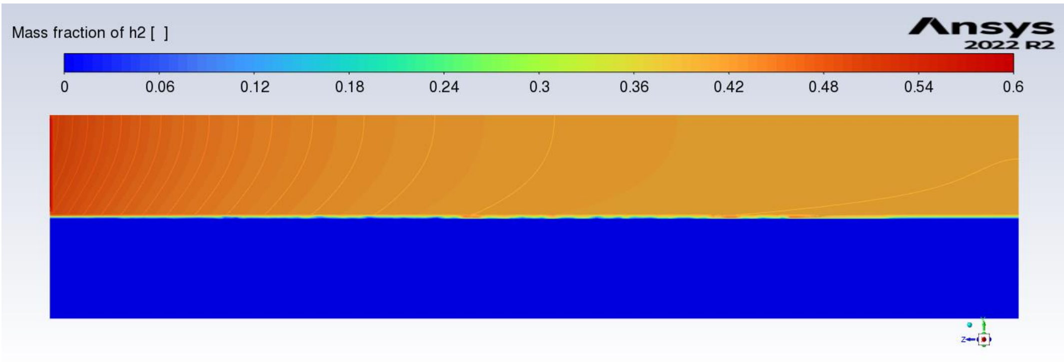

Fig. 10. Mass fraction of h2 on the plane of symmetry at the cathode and anode for 0.006 μg/s

Fig. 11 shows the content of hydrogen in the channels for a mass flow rate of 0.0008 μg/s, which is over 1000 times less. Here, finally, there is a significant decrease in the hydrogen content in the anode channel compared to the previous cases. Almost all of the hydrogen reacted and dropped from 0.6 at the beginning of the channel to about 0.15. For this value of mass flow rate, the current generated in the cell is 0.635 A/cm^2, which is still a lot. Therefore, as it has already been said, it is very important to choose the right proportion of fuel and this task depends on the type of cells and, of course, on the shape of the channels distributing hydrogen on the surface of the membrane. It should be remembered, that an important factor regulating the efficiency and life of the fuel cell is the appropriate humidity, which also depends on the stoichiometric proportion of the supplied factors (Liu et al., 2022; Cheng et al., 2021; Kim, 2012).

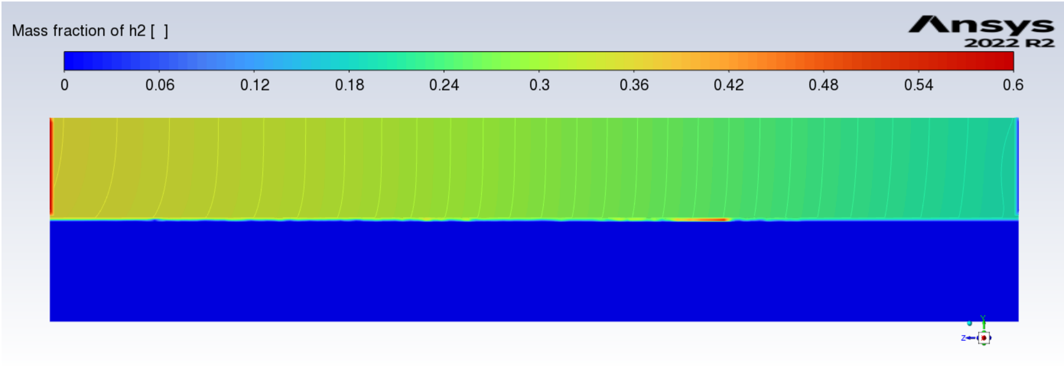

Fig. 11. Mass fraction of h2 on the plane of symmetry at the cathode and anode for 0.0008 µg/s

Summing up the performed analyses, it can be concluded that despite the huge change in the amount of fuel supplied, there was no significant decrease in the value of the generated current. This means, that it is a huge challenge to achieve proper mixing of the reactants in the fuel cell. For example, in work (Liu et al., 2022) there is a proposition of using a dual-ejector system, which is quite interesting, but according to the authors' suggestion, a very good idea for such a process is to force a turbulent flow in all channels of the fuel cell.

4. CONCLUSIONS

During the work described in the paper ANSYS software was used; which has already proven to be a very useful tool in many scientific works; to analyze the rather complicated flow existing in PEMFC. This is a quite new approach to using the capabilities of this software. As a result of the numerical analyses of the effect of the amount of fuel supplied on the operation of the PEMFC, a very obvious conclusion was obtained, that increasing the amount of hydrogen in the system generates a higher current. But on the other hand, a very interesting feature was noticed, that a very large change in the amount of fuel supplied does not cause a very drastic decrease in the value of the current generated by the fuel cell. This, of course, is related to what was mentioned earlier in the work, that the problem of mixing fluid layers in the channels supplying both hydrogen and oxygen plays a very important role. The flow generally is laminar and there is no strong mixing of the fluid layers and a lot of hydrogen is not led to the reaction, which generates huge losses.

From the fact that for the mass flux of $9 \cdot 10^{-1}$ µg/s the current value is 0.675 A/cm^2 and for the flux of $8 \cdot 10^{-4}$ µg/s the current is 0.635 A/cm^2, it is very clear that current drop is 0.04 A/cm^2, which is only 5.926% of the original value, whereas the amount of supplied hydrogen is a thousand times lower. Therefore, it is very important to properly power the fuel cells in such a way as to obtain stoichiometric conditions, which is certainly not an easy process.

The type of flow in the supply channels seems to be very important here. Many works focus on the shape and number of the channels themselves, but an attempt to turbulize the flow in these channels also seems very accurate. According to the authors, great effort should be put into designing channels in such a way as to generate turbulent flow in them. This will significantly increase the efficiency of fuel cells without the need for extension of the channels, and thus the size of the entire cell. Such analyzes will be undertaken in subsequent works.

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