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INVESTIGATION OF THE FUEL CELL TEMPERATURE DISTRIBUTION ON THE CURRENT DENSITY AND ELECTRIC POTENTIAL FIELDS

In many medical systems a reliable energy sources play an important role. In the case of failure of external energy system, the local electrical supply has to be activated. Such electrical sources should be environmentally friendly, infallible and easy in usage. The fuel cells using hydrogen as an energy source fulfil these conditions. Numerical modelling of such electrical sources is the primary aim of this publication. Influence of the distribution of temperature on the current density and electric potential fields in electrode of the PEM fuel cell is thoroughly considered. The problem is stated as coupled field problem, where partial differential equations describing mass transport are coupled with Laplace equations describing electric potential and temperature distribution. At the end some illustrative example is given

1. INTRODUCTION

In medical systems, reliability of energy sources is of primary importance. The failure of electrical sources can cause serious consequences for the health of patients. The power needed can change from many megawatts in the case of energy systems for hospitals, to less then one watt in the case of devices grafted into human body. Not only reliability but also a long period of operation is very important. Such energy sources as battery grafted into human body have to be change after some period of time, what usually require chirurgical operation.

Fuel cells are energy sources, which in many aspects fulfil these requirements. They can be supplied with hydrogen and as result of energetic reactions deliver clean water, or in the case of electrical sources implanted into human body can use sugar occurring in human blood as energy source. The range of potential applications of fuel cells in practical medicine is enormous and with further development of these sources will in future substantially increases.

The proton exchange membrane (PEM) fuel cell consists of two gas diffusion layers (GDL) separated by PEM. Thin platinum catalyst layer is located between each GDL and PEM. The diffusion layer plays very important role in overall performance of fuel cell because it transports reactant species to reaction sites and carries away electrochemical reaction products, heat and current density. Numerical simulation of all aspects of GDL performance is very important from practical point of view because most of the working parameters are very difficult to measure. This is mainly caused by the very little cross dimension of single cell. Typical electrodes are made of

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carbon fibre paper which in turns is made of single carbon fibres. Because of this GDL diffusion and convection coefficients are not constants numbers but have tensor values.

The gas diffusion layer (GDL) is part of fuel cell where reactants lead the reaction sites and which way reaction products leave out the electrodes. There are two distinct mechanisms, which are responsible for species transport. The convection of the gas species is caused by pressure difference and diffusion is affected by gas component concentration differences. Let us consider cathode of the PEM fuel cell. This electrode contacts from polymer electrolyte side a catalyst layer, which is a very thin film of pure platinum, and from other side interdigitated gas distributor (IGD). It is made usually from graphite plate and its main function is to supply to the GDL gas mixture and carrying away a heat and generated current [1]. Because of the geometrical symmetry only a part of the GDL needs to be considered (fig. 1).

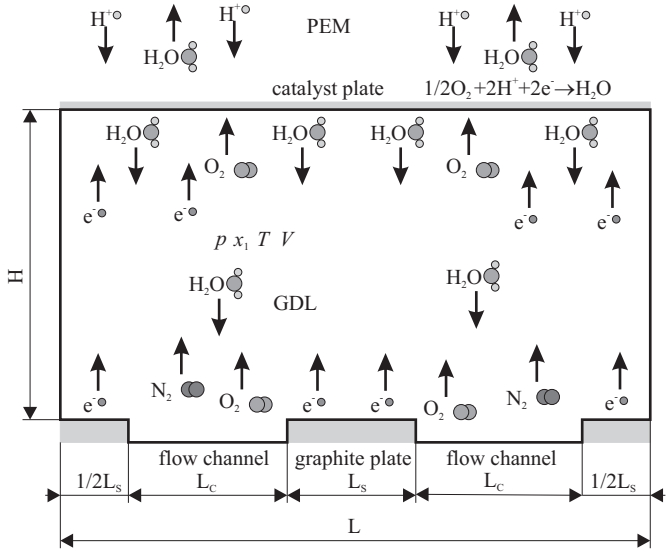

Fig. 1. Model of the PEM fuel cell cathode.

2. MAIN EQUATIONS

The model of the GDL with variable temperature bases on equations describing multicomponent mass transport. For simplified Fickian model of the mass transport we get four nonlinear partial differential equations mutually coupled not only directly but also through boundary condition [3]. The independent variables are pressure p, molar fraction of the oxygen x_1, electric potential φ and the temperature T. From the Darcy's and mass conservation laws we get:

$$-\frac{k_{\mathrm{p}}}{\varepsilon_{\mathrm{p}}\mu}\nabla\cdot\left(C\nabla p\right)=0 \tag{1}$$

where C is molar concentration of the gas mixture, k_{p} is hydraulic permeability, ε is porosity and μ is viscosity of the GDL [2].

Assuming ideal gas equation:

$$p=CRT \tag{2}$$

where R is gas constant, we get first partial differential equation for pressure p:

$$-\frac{k_{\mathrm{p}}}{\varepsilon_{\mathrm{p}}\mu RT}\left[p\nabla^2 p+\nabla p\cdot\nabla p-\frac{p}{T}\nabla p\cdot\nabla T\right]=0 \tag{3}$$

The mass conservation law for the oxygen can be formulated as follow:

$$\nabla\cdot\left(-DC\nabla x_1+C\,x_1\mathbf{U}\right)=0 \tag{4}$$

where D is diffusion coefficient and $\mathbf{U}$ is vector of molar average velocity. Assuming Darcy's law:

$$\mathbf{U}=-\frac{k_{\mathrm{p}}RT}{\varepsilon_{\mathrm{p}}\mu}\nabla C \tag{5}$$

we get second equation for molar fraction of the oxygen x_1:

$$-\frac{D}{R}\left(\frac{p}{T}\nabla^2 x_1+\nabla x_1\cdot\nabla\frac{p}{T}\right)-\frac{k_{\mathrm{p}}}{\varepsilon_{\mathrm{p}}\mu R}\left[x_1\nabla\left(\frac{p}{T}\nabla p\right)+\frac{p}{T}\nabla p\cdot\nabla x_1\right]=0 \tag{6}$$

Finally, after some manipulations we get second partial differential equations:

$$-\frac{Dp}{RT}\left(\nabla^2 x_1+\frac{D\,\varepsilon_{\mathrm{p}}\mu+k_{\mathrm{p}}p}{pD\,\varepsilon_{\mathrm{p}}\mu}\nabla p\cdot\nabla x_1-\frac{1}{T}\nabla x_1\cdot\nabla T\right)=0 \tag{7}$$

According to the Fourier's law flux of the heat $\mathbf{q}$ is proportional to the gradient of the temperature [5]:

$$\mathbf{q}=-\lambda\nabla T \tag{8}$$

where λ is a heat transfer coefficient. The only heat exhaled inside the GDL is the result of Ohmic loses, thus:

$$\nabla\cdot\mathbf{q}=\sigma\nabla\varphi\cdot\nabla\varphi \tag{9}$$

So, finally, third partial differential equation for temperature T is:

$$\nabla\cdot\left(-\lambda\nabla T\right)=\sigma\nabla\varphi\cdot\nabla\varphi \tag{10}$$

In the GDL current density vector $\mathbf{j}$ has to fulfil Lapalce equation [4]:

$$\nabla\cdot\mathbf{j}=0 \tag{11}$$

On the second hand the current density vector can be obtain from the Ohm's law:

$$\mathbf{j}=-\sigma\nabla\varphi \tag{12}$$

where σ is the electron conductivity of the GDL. The forth partial differential equation describing electric potential distribution can be formulated as:

$$\nabla \cdot \left(-\sigma \nabla \varphi \right) = 0 \tag{13}$$

3. BOUNDARY CONDITIONS

On problem boundary each molar concentration has to fulfil adequate Dirichlet or Neumann boundary conditions.

Section I – Graphite plate

Along this part of boundary graphite plate is in contact with carbon fibre material and throughout this section can be no flux of any species. Because fluxes of all species at this boundary section are parallel to the boundary surface, the fluxes entering the graphite plate are equal zero.

$$\frac{\partial p}{\partial n} = 0 \quad \text{and} \quad \frac{\partial x_1}{\partial n} = 0 \tag{14}$$

The pressure and electric potential is given by Dirichlet's conditions as follows:

$$T = T_{\mathrm{g}} \quad \text{and} \quad \varphi = \varphi_{\mathrm{e}} \tag{15}$$

Section II –Flow channels

On this part of the boundary fibrous carbon material contacts with flow channel and here reactant species enter the anode. This results following Dirichlet's conditions:

$$p = p_{\mathrm{g}} = \frac{C_{\mathrm{g}}}{RT_{\mathrm{c}}} \quad \text{and} \quad x_1 = x_{1\mathrm{g}} \tag{16}$$

The normal partial derivate of the electrical potential is equal zero. The heat is lead out through flow channel together with exhaust gases, so on this boundary temperature has to fulfil following Neumann's condition:

$$\frac{\partial T}{\partial n} = \lambda \left(T - T_{\mathrm{c}} \right) \tag{17}$$

Section III – Left and right sides of the calculation domain

We assume that solution is periodic with respect to the calculation variables and thus all fluxes are directed parallel to the y axis. This causes that boundary conditions in this section are the same as for section I. This means that normal components of fluxes and electrical potential on these parts of boundaries are equal zero.

Section IV– Platinum catalyst layer

The most complicated dependencies between variables are in the boundary conditions on the catalyst layer, where the electrochemical reaction takes place. The electrochemical reaction is the main source of heat and the only source of the electric current.

The fluxes of first $\mathbf{N}_1$ and second $\mathbf{N}_2$ gas component have to fulfil following equations:

$$\mathbf{N}_1 \cdot \mathbf{n} = \frac{j}{4F} \quad and \quad \mathbf{N}_2 \cdot \mathbf{n} = \alpha \frac{j}{2F} \tag{18}$$

Normal derivate to the boundary of the current density can be obtained from Buttler-Volmer equation as:

$$j = \frac{a x_1 p}{RT} \exp\left(\frac{4kF}{RT}\eta\right) \tag{19}$$

thus, the Neumann's boundary conditions for pressure and molar fraction of the first component are:

$$\frac{\partial p}{\partial n} = -\frac{(1+2\alpha)\,\varepsilon_p \mu\, a\, x_1}{4F\, k_p \gamma_r} \exp\left(\frac{4kF}{RT}\eta\right) \tag{20}$$

and

$$\frac{\partial x_1}{\partial n} = -\frac{a\, x_1 \left[\gamma_r - x_1(1+2\alpha)\right]}{4FD\gamma_r} \exp\left(\frac{4kF}{RT}\eta\right) \tag{21}$$

The Neumann's boundary condition for the electrical potential φ can be calculated as:

$$\frac{\partial \varphi}{\partial n} = \frac{j}{\sigma} = \frac{a x_1 p}{\sigma RT} \exp\left(\frac{4kF}{RT}\eta\right) \tag{22}$$

We assume the temperature of the GDL – membrane interface as:

$$T = T_m \tag{23}$$

4. AN ILLUSTRATIVE EXAMPLE

In the illustrative example the dependence between temperature of the GDL and the electric potential and current density distribution is researched. In the fig. 2 distribution of the electric potential is shown. The reference potential of the graphite plates is equal zero. In the fig. 3 current density vector inside the GDL is drawn. One can see that only at the graphite plates current density flux is flowing into the IGD and next to the external load.

In the figures 4 and 5 dependencies between electric potential and the normal derivate of the current density vector on the catalyst layer for different values of temperature are drawn. Because of ohmic's loses higher values of the potential and current density are for lower temperature of the GDL. The results of the simulation show, that heat management in the fuel cell, especially in stack of the cells is very important from the practical point of view and has a great influence to the performance of the fuel cell system.

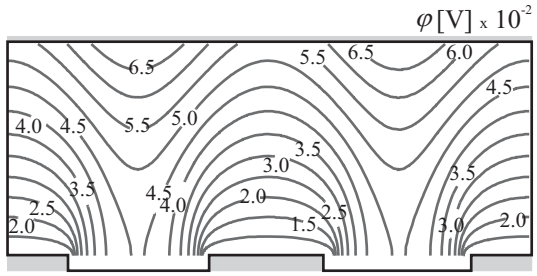

Fig. 2. Distribution of the electric potential in the cathode of the PEM fuel cell.

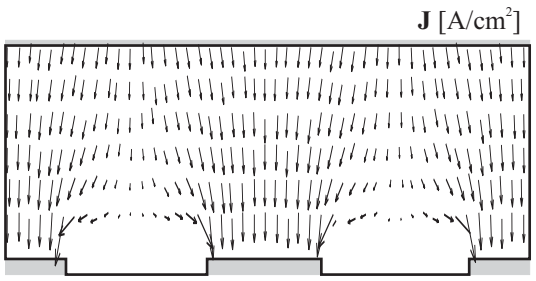

Fig. 3. Distribution of the current density in the cathode of the PEM fuel cell.

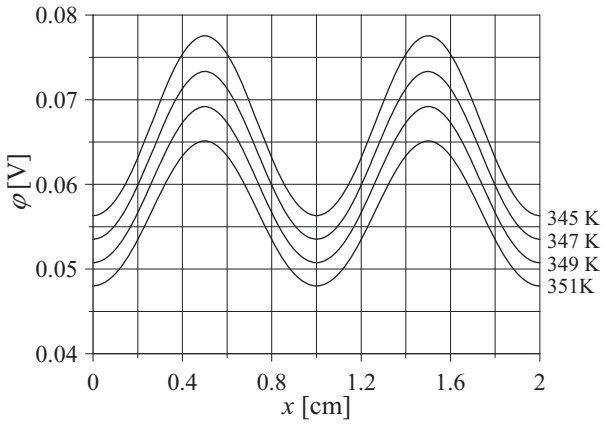

Fig. 4. Dependency between electric potential distribution V and the temperature on the catalyst layer.

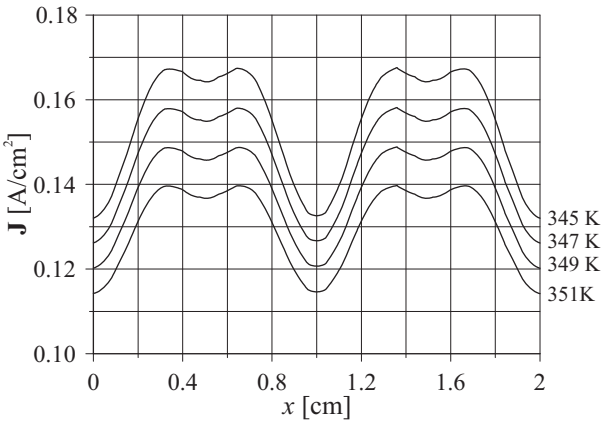

Fig. 5. Dependency between distribution of the normal component of current density vector **J** and the temperature on the catalyst layer.

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