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TRANSPORT OF GAS COMPONENTS IN THE CATHODE OF PEM FUEL CELL

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Abstract: Simulation of the performance of the PEM fuel cell based on the fluid flow approach in electrodes of the proton exchange fuel cell is developed. Gas mixture transport from flow channel to catalyst layer based on Darcy's law, Fick's law and ideal gas law is developed. As field variables both concentrations of hydrogen and water vapour where chosen. As a result, mutually coupled nonlinear partial differential equations were obtained. These equations where solved using standard finite element method in two dimensions.

Keywords: PEM fuel cells, mass transport, finite element method.

1 Introduction

A critical component of such fuel cells is the electrode, known as a gas diffusion layer (GDL), which is a very thin layer of porous carbon fibre paper lying between platinum catalyst layer from one side and gas distribution layer form the other. The flow of gas mixture in the GDL is governed by the convection law, which governs the motion of the gas species through the porous medium caused by pressure gradients, and multicomponent diffusion of the reacting and nonreacting gas species caused by concentration gradients, relative to the convection velocity [1].

In this paper, a gas mixture model is developed to study air and water vapour flow in cathode of the PEM fuel cell. It is based on the same theoretical considerations as in papers [2,4], but uses finite element method to discretize resulting nonlinear set of equations. It extends results presented in these papers using directly hydrogen and water vapour concentrations C_1 and C_2. At the end some illustrative example is given.

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2 Main equations

We assume that gas mixture in flow channel is composed from three components: oxygen with concentration C_1, water vapor with molar concentration C_2 and nitrogen N_2 which concentration is assumed C_3.

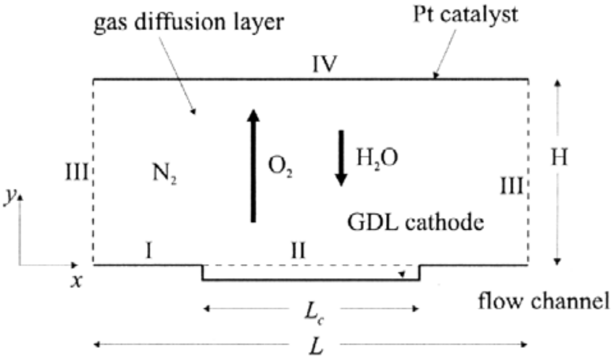

Fig.1. Gas diffusion layer together with flow channel and catalyst layer.

The total gas concentration is denoted by C and is equal [3]:

$$C = C_1 + C_2 + C_3 \tag{1}$$

We assume further that vapour concentration is a fixed part of the total concentration C which is equal $(1 - \gamma r)C$, thus:

$$C = C_1 + C_2 + (1 - \gamma_r)C \tag{2}$$

Because only three variables C_1, C_2 and C change their values and they are mutually related by (1), only two of them are to be chosen independently. As unknown variables we assume oxygen concentration C_1 and water vapour concentration C_2. Every mixture component for $i = 1, 2, 3$ also has to fulfill mass conservation low:

$$\nabla \cdot \left(C_i \, \mathbf{U} + \mathbf{J}_i \right) = 0 \tag{3}$$

where $\mathbf{J}_i$ is the diffusive flux measured relative to the molar averaged velocity $\mathbf{U}$. The total convective and diffusive flux of this component with respect to static or laboratory coordinates takes the form:

$$\mathbf{N}_i = C_i \, \mathbf{U}_i = C_i \, \mathbf{U} + \mathbf{J}_i \tag{4}$$

The diffusive flux of any gaseous component $\mathbf{J}_i$ is given by Fick's law, which states that molar flux of this component is relative to the molar-averaged velocity and is proportional to the gradient of the mole fraction C_i/C according with relation [5]:

$$\mathbf{J}_i = C_i \left(\mathbf{U}_i - \mathbf{U} \right) = -DC\nabla\left(\frac{C_i}{C} \right) \tag{5}$$

where coefficient D is the diffusivity and usually has dimension cm^2/s. The mixture velocity $\mathbf{U}$ with which all species are moving is given by Dercy's law and depends on pressure gradient:

$$\mathbf{U} = -\frac{K}{\varepsilon_p \mu} \nabla(P) = -\frac{K\,RT}{\varepsilon_p \mu} \nabla(C) \tag{6}$$

where μ is the viscosity of the mixture and characterizes gas properties, while anode material properties are described by permeability K and porosity ε_p. The last relation between pressure and mixture molar concentration C is given by state (constitutive) equation for the gases. Assuming that coefficient Γ is given by:

$$\Gamma = -\frac{K\,RT}{\varepsilon_p \mu} \tag{7}$$

we get

$$\mathbf{U} = -\Gamma \nabla(C) \tag{8}$$

After assumption that gas is ideal and adiabatic, the pressure P depends linearly from overall species concentration:

$$P = RT\,C \tag{9}$$

where R is the universal gas constant and T is the temperature. Introducing this equation int

$$\nabla \cdot \left(\Gamma C \nabla(C) \right) = 0 \tag{10}$$

This is the first partial differential equation for C variable. The second equation can be derived from the molar conservation law for oxygen (3):

$$\nabla \cdot \mathbf{N}_1 = 0 \tag{11}$$

where molar flux of the oxygen $\mathbf{N}_1$ is relative to the laboratory-fixed coordinate reference system:

$$\Gamma \nabla \cdot \left(C_1 \nabla C \right) + D_1 \nabla \cdot \left[C \nabla \left(\frac{C_1}{C} \right) \right] = 0 \tag{12}$$

Solving the above two equations with respect to variables C_1 and C_2 we get:

$$\nabla^2 C_1 = -\left(\frac{2}{(C_1 + C_2)} - \frac{\Gamma}{\gamma_r D_1} \right) \left(\frac{C_1}{(C_1 + C_2)} \right) \left(\nabla (C_1 + C_2) \right)^2 - \left(\frac{\Gamma}{\gamma_r D_1} - \frac{1}{(C_1 + C_2)} \right) \nabla C_1 \cdot \nabla (C_1 + C_2) \tag{13}$$

and

$$\nabla^2 C_2 = \left[\frac{C_1 - C_2}{C_1 + C_2} - \frac{\Gamma C_1}{\gamma_r D_1}\right]\frac{1}{(C_1 + C_2)}\left(\nabla(C_1 + C_2)\right)^2 + \left(\frac{\Gamma}{\gamma_r D_1} - \frac{1}{(C_1 + C_2)}\right)\nabla C_1 \cdot \nabla(C_1 + C_2) \quad (14)$$

The two above highly nonlinear and mutually coupled partial differential equations should be solved together with appropriate boundary conditions. On the part of the boundary where fibrous carbon material contacts with flow channel reactant species enter the anode. For all points on this part of the boundary $C = C_{\mathrm{g}}$ and has constant and prescribed value. This leads to the condition on water vapour concentration value:

$$C_{2\mathrm{g}} = \gamma_r C_{\mathrm{g}} - \gamma C_{\mathrm{g}} = (\gamma_r - \gamma) C_{\mathrm{g}} \quad (15)$$

In analogous way we can derive Neumann's boundary condition for C_1:

$$\frac{\partial C_1}{\partial n} = \frac{r_0}{D_1}\left(C_{1g} - C_1\right) \quad (16)$$

On the catalyst layer on the other hand we have

$$\frac{\partial C_1}{\partial n} = -\frac{r_H C_1}{D} - \frac{\gamma_r \nu r_H C_1^2}{\Gamma(C_1 + C_2)\left((1-\nu)C_1 + C_2\right)} \quad (17)$$

$$\frac{\partial C_2}{\partial n} = r_H\left(\gamma_r C - C_2\right)\left[\frac{1}{D} - \frac{\nu C_2}{\Gamma C\left[(1-\nu)\gamma_r C + \nu C_2\right]}\right] \quad (18)$$

Equations (13) and (14) together with Dirichlet's and Neumann's boundary conditions (15) – (18) were solved by standard finite element method [6,7].

3 An illustrative example

Values of the constants and the geometry of the GDL cathode are given in [3] and will be not repeated here. The numerical calculations are consistent with theoretical considerations. At the figures 2 and 3 we can see fluxes of the flows of the gas components at the GDL cathode.

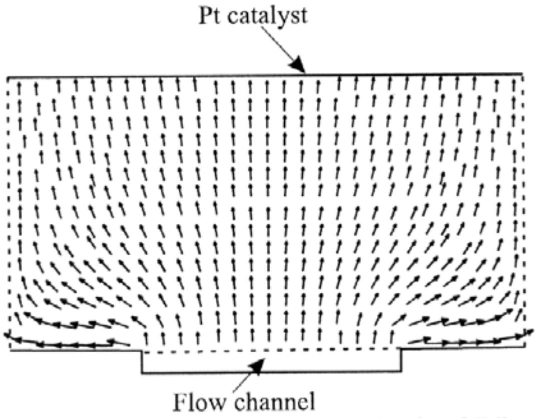

Fig.2. Flux of the flow of the oxygen in the GDL cathode.

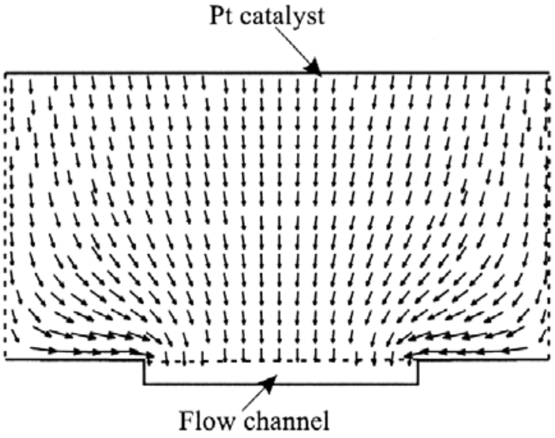

Fig.3.Flux of the flow of the vapor water in the GDL cathode.

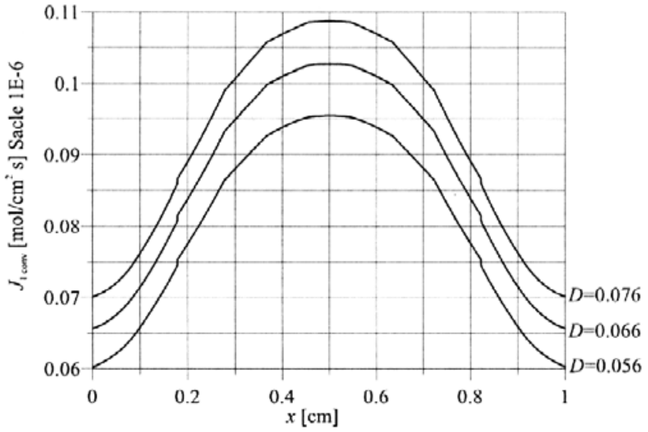

Fig. 4. Convection flow of the oxygen along the GDL cathode.

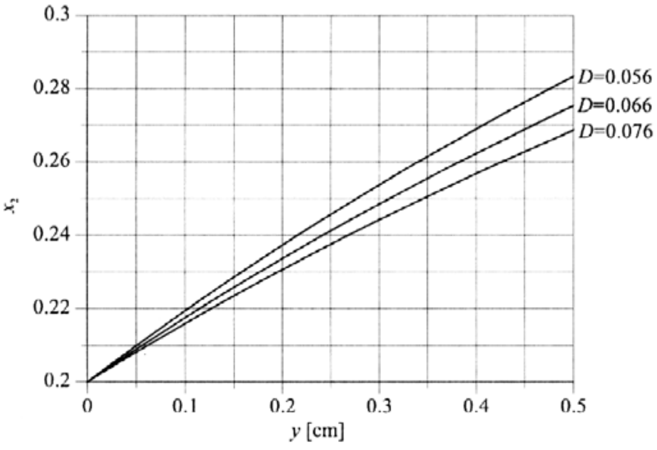

Fig.5. Molar fraction of the vapor water across the GDL cathode.

At the figure 4 we can see flux of the convection flow of the oxygen along the GDL anode in the middle between flow channel and catalyst layer (y = 0.5H). We can observe the dependence between diffusivity parameter D of the GDL cathode and the value of the flow. We can see that for greater cathode diffusivity D the amount of the oxygen, which reaches through cathode, is greater.

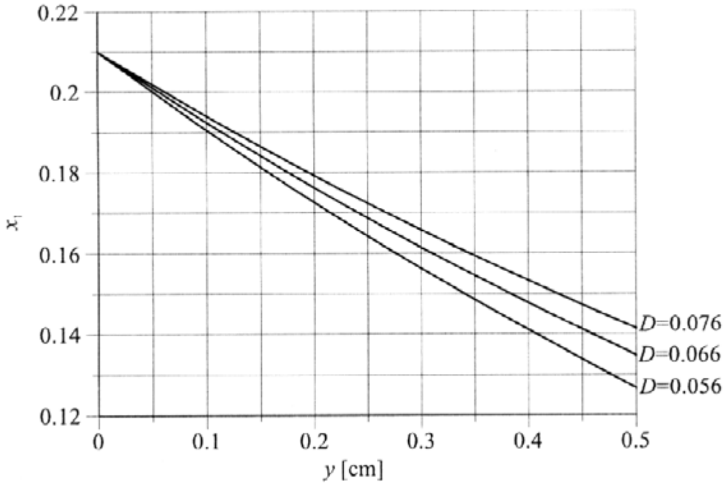

Fig. 6. Molar fraction of the oxygen across the GDL cathode.

At the figures 5 and 6 we can see the molar fraction of the gas components across the cathode calculated at x = 0.5L. The molar fraction of each of the component is defined as $x_i = C_i/C_g$. We can see that for greater cathode diffusivity D the amount of the oxygen, which reaches of the catalyst layer, is greater and therefore electrochemical reaction intensity also increases.

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