

Modeling of flow and transport processes occurred in a typical polymer electrolyte membrane fuel cell (PEMFC)

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Abstract. In the present work, a three dimensional model examining the fluid flow along with the fundamental transport phenomena occurring in a typical polymer electrolyte fuel cell (PEMFC), i.e. heat transfer, mass transport and charge transfer, has been developed. The flow field was simulated according to the well known Navier-Stokes equations, while the heat transfer was described by the typical conduction/convection equation and the mass transport by the convection/diffusion one. Furthermore, reaction kinetics were studied by the Butler-Volmer equation for the heterogeneous reactions occurring at the porous electrodes. The developed model was numerically solved by using the commercially available CFD package CFD-RC[®], which is based on the multi-step finite volume method. The fuel cell performance in terms of velocity, temperature, mass fractions of active compounds and electric field has been investigated as well.

Introduction

Fuel cell systems are energy devices that directly convert the chemical energy of the feeding fuel into electricity without Carnot limitation, being suitable for stationary and mobile applications. Due to the high conversion efficiencies and the negligible environmental impact, fuel cell technology is considered as one of the most promising to contribute essentially to generation of electrical power in the near future [1,2]. Polymer Electrolyte Membrane fuel cells (PEMFCs) have high power densities, quick start-up and load characteristics while their normal operational temperature is quite low, thus they gain significant interest among the researchers [3]. For decades, several studies focus on modeling in order to obtain a deep insight on their performance characteristics and improve their reliability and their cost-effectiveness as well [4-6].

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Theoretical background

In the present study, a typical polymer electrolyte membrane fuel cell (PEMFC) consisting of an anode and a cathode compartment separated by a membrane and surrounded by two current collectors was modeled. The humid air flows in the cathode gas channel, while the gas mixture enters the anode compartment of the fuel cell. It was also assumed that electrochemical reactions take place only in the porous electrodes, while no other bulk reaction occurs either on porous media or in bulk phase. By referring to one electron (e^-) basis, the electrochemical reaction considered to occur at the porous anode is as follows:



The necessary protons are provided by the electrochemical reaction taking place in the porous cathode electrode:



The Navier-Stokes equation can adequately describe the steady state laminar flow for compressible fluids as:

$$\underline{u} \cdot \nabla (\rho \underline{u}) = -\nabla p + \mu (\nabla^2 \underline{u}) \quad (3)$$

where \underline{u} is the velocity vector, ρ is the density, p is the pressure, and μ is the viscosity.

By neglecting radiation effects, the steady state heat transfer equation for temperature, T , is given as follows:

$$\underline{u} \cdot \nabla (\rho c_p T) = \dot{Q} + [\nabla \cdot a \nabla (\rho c_p T)] - (\rho c_p T) \nabla \cdot \underline{u} \quad (4)$$

where c_p is the mixture's specific heat, a is the diffusion thermal coefficient, \dot{Q} is the produced/ consumed heat due to the exothermic/endothermic reactions taking place at porous electrodes. Furthermore, Joule heating and electric work appears at the electrodes, so these additional terms have been incorporated in \dot{Q} while solving the above equation inside the porous media.

Mass transport equation for each species has also to be solved for the calculation of species concentration, C_i and it can be written as follows:

$$\underline{u} \cdot \nabla C_i = \nabla \cdot (D_{i,mix} \nabla C_i) + \dot{\omega} \quad (5)$$

where $D_{i,mix}$ is the diffusion coefficient of i species in the mixture and $\dot{\omega}$ is the production/destruction rate of the i -th species in the gas phase.

Finally, the current density is defined through the typical Butler-Volmer expression, assuming that the electrode processes are solely controlled by charge transfer.

$$j = j_0 \left[\exp\left(\frac{a_a F}{RT} \eta\right) - \exp\left(-\frac{a_c F}{RT} \eta\right) \right] \quad (6)$$

where j_0 is the exchange current density at a known open circuit voltage, a_a and a_c are the anodic and cathodic charge transfer coefficients, respectively, determined by the Tafel plots, F is the Faraday constant, R is the ideal gas constant and η is the electrode overpotential.

Proposed model

Geometry and general

The geometrical characteristics of the modeled fuel cell consisting of seven separate regions, the anode and the cathode channel, the porous anode and cathode, the membrane and the two contacts are presented in Figure 1, whose dimensions are according to Ramakrishna et al. [7]. Humid air (23.5 % O₂, 75 % N₂ and 1.5 % H₂O) and fuel mixture (73 % H₂, 27 % H₂O) were introduced into the cell through the air channel and fuel channel respectively. The diffused H₂ and O₂ species into the porous electrodes participate in the involving electrochemical reactions, while the non reacted species exit the fuel cell channels. Membrane separates the fuel and air mixture and simultaneously it is a medium through which the produced protons ions migrate from anode to cathode in order to participate in the reaction. Finally, two current collectors where the voltage is usually applied were placed at the surroundings of the fuel and air channel.

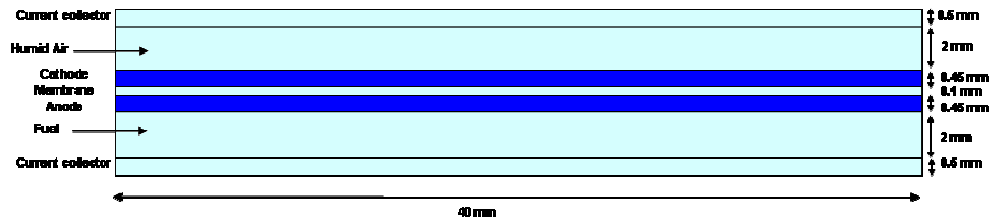


Figure 1: Simulated cell geometry.

Materials

Both air electrode (cathode) and fuel one (anode) were simulated as isotropic porous media and their basic properties are listed in Table 1. Also, a thermodynamically optimal proton conductor was considered for the membrane and its basic porous media characteristics are also presented in Table 1. Additionally, for the basic properties of the gas phase, the density is estimated by the Ideal Gas Law, the viscosity by the Mix kinetic theory, the specific heat by adjusting the JANNAF curves, the thermal conductivity by the Prandtl number ($Pr=0.707$) and the mass diffusivity by the Schmidt number ($SCH=0.7$). In addition, both the gas phases are considered not electrically conductive,

thus the fluid electric conductivity for them was set to $1e^{-20} \Omega^{-1} m^{-1}$. Finally, for the electrochemical reactions the reference current transfer values used for the Butler-Volmer equation were $j_0 = 9.2 \cdot 10^8 \text{ Am}^{-3}$ and $j_0 = 1.05 \cdot 10^6 \text{ Am}^{-3}$ for the fuel and air electrode reactions, respectively. Accordingly, the charge transfer coefficients imposed were $a_a = a_c = 0.5$ [4] for the anode electrode and $a_a = a_c = 1.5$ [8] for the cathode electrode.

Table 1. Porous media characteristics.

Compartments	Anode	Membrane	Cathode
porosity, ε (fluid volume/total volume) [8]	0.40	0.28	0.40
permeability, κ (m^2) [4]	$1e^{-11}$	$1e^{-11}$	$1e^{-11}$
pore size, d_p (m)	$1.5e^{-6}$	$1e^{-6}$	$1.5e^{-6}$
solid thermal conductivity, k_s ($W m^{-1} K^{-1}$) [4]	150	0.95	150
surface to volume ratio, S/V (m^{-1})	1000	-	1000
solid electric conductivity, σ_s ($\Omega^{-1} m^{-1}$) [4]	53	$1e^{-20}$	53
fluid electric conductivity, σ_f ($\Omega^{-1} m^{-1}$)	4.2	By membrane model	4.2

Boundary conditions

Obviously, the above differential equations should be integrated along with the appropriate boundary conditions, which depend on each specific application. Constant values of mass flows rates at the inlets of gas channels were applied for the homogeneous mixtures. Specifically, the mixture's mass flow rate at the anode channel was set to $0.8 \times 10^{-6} \text{ kg/s}$ and at the cathode channel mixture at $1.1 \times 10^{-6} \text{ kg/s}$, imposing flow conditions that assure an overall temperature gradient less than 100K. For the gas channels, non-slip boundary condition was set to the walls, while fixed pressure boundary condition of 1 atm was set to the two outlets [4]. It was assumed that there is no mass accumulation and consequently zero mass flux was imposed to the walls and to the exits as well. Both air and fuel mixtures were considered isothermal and were preheated before entering the fuel cell at 353K (constant), while zero heat flux was set to all the other boundaries. Fixed potential of -0.6V was set to the cathode contact (working electrode) and 0V at anode contact (counter electrode) respectively [4, 9], while zero current density was applied to the fluid phase of the porous media. Finally, for the symmetrical walls zero-gradient boundary conditions were applied.

3.4 Numerics

In order to eliminate the computational time, only the half geometry of the 3-D original plane was simulated, since symmetry around the central plane of the original planar fuel cell exists. The finite volume method was used to integrate the system, being applicable through the commercially available CFD-RC[©] software package. The simulated symmetrical geometry was discretized in space by a structure grid consisting of 19494 cells (see Figure 2). Residual values lower than 10^{-4} were achieved for all the unknown quantities.

4. Results and discussion

The performance of the PEM fuel cell can be well described by the microscopic results regarding velocity, temperature and electric potential. Additionally, the variation of species composition, along x-dimension, of the fuel cell was obtained.

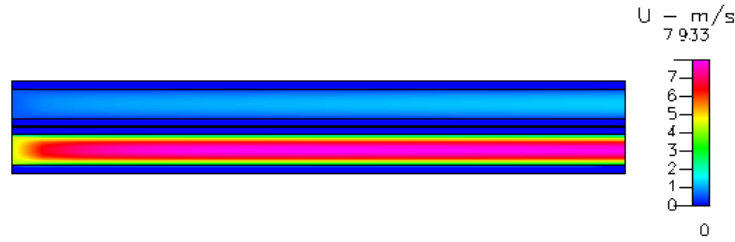


Figure 2: Velocity field

The velocity profile for the planar PEM fuel cell is imprinted in Figure 2. The developed velocity profile at the anode and cathode channel is obviously parabolic, while the velocity on the walls is zero, satisfying the non slip boundary condition. The hydrogen and water mass fraction along the feed stream direction and at the middle of anode and cathode electrodes, respectively, are presented in Figures 3a & 3b, where a decrease in hydrogen mass fraction is clearly depicted in the anode compartment, accompanied by a consequent increase of steam in the cathode compartment. This behavior of mass fractions is an expected outcome due to the heterogeneous electrochemical reactions occurred in the fuel cell. A certain amount of heat is produced in the porous cathode, due to the exothermicity of the reaction (2), being spatially transferred due to convection and diffusion.

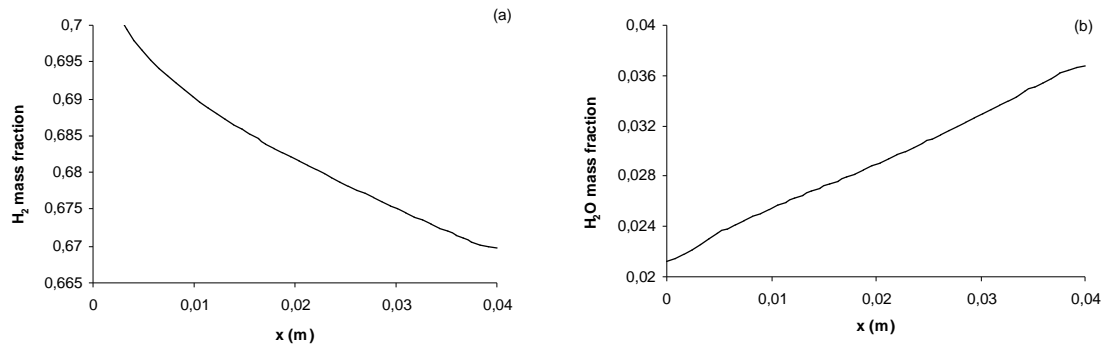


Figure 3: Spatial mass fraction distribution: H₂ at middle of anode (a) and H₂O at middle of cathode (b)

Figure 4 shows the temperature distribution, which becomes higher towards the outlet area. This gradually increasing heat production is a presumable result of the analogous fuel consumption, due to the diffusive regime. It is also obvious that convective effects prevail at the air and fuel channel due to the velocities developed and as a result temperature at the inlet of these channels is smaller. Finally, the electric potential output is depicted in Figure 5, where slightly uniform profile of low values of electric potential are obtained at anode and cathode electrode. This behavior can be attributed to the low operational temperature of PEM, which corresponds to subsequent low energetic content of feedstream, thus to lower electrical power produced.

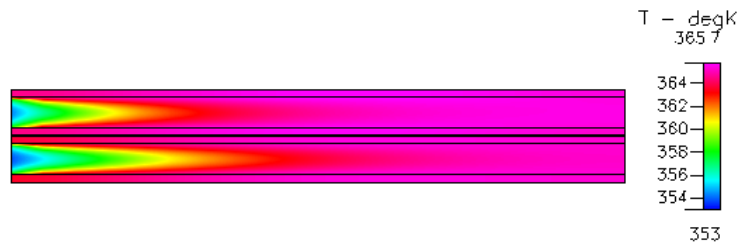


Figure 4: Temperature distribution in the cell

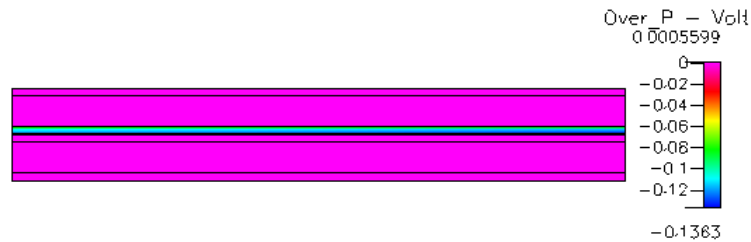


Figure 5: Overpotential profile in the cell

Conclusions

The developed model seems to be sufficient enough to qualitatively describe the operation of a PEMFC in terms of microscopic transport phenomena and for constant conditions the velocity field, the temperature variation, the mass fractions of active components and electric field are obtained. Temperature profile follows the spatial variation of consumption/production of active compounds, while overpotential presents a slightly uniform profile with very low values.

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