INVESTIGATION AND MODELING OF THE FLOW FIELD IN SOFC

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ABSTRACT

The solid oxide fuel cells produced by VPS-Technology have been investigated in this work. Using the thin film concept, various anode substrates were tested. At first, the relevant transport processes were experimentally studied under operating conditions if possible. These processes are the flow in gas channels, and the gas permeation through and the diffusion in the functional layers, respectively. A mathematical 3-D model has been developed to simulate the flow field distribution, and the numerical calculations have been implemented using the CFD program Star CD. The 3-dimensional flow distribution has been studied using laminar and turbulence models. Furthermore, the experimentally determined parameters were used into the porous model, and the influence of the porous structure on the distribution of flow investigated.

INTRODUCTION

A solid oxide fuel cell for an on-board Auxiliary Power Unit (APU) for mobile applications is being developed by the BMW Group and a number of partners from industry and research institutes, as reported in (1). Here, we discuss one approach based on thin film concept developed at DLR, Stuttgart (2). In this planar concept, metallic bipolar interconnector and vacuum plasma sprayed electrodes and electrolyte supported by a metallic substrate are used.

The performance of SOFC is not only a function of operating conditions like temperature, pressure and the fuel gas composition, but also strongly dependent on the mass transport such as the flow field in the gas channels, gas permeation and diffusion in porous functional layers. A bad distribution of reactants among the gas channels, for example, can lead to several problems: lower electrical power output, thermal stresses and damage to electrodes due to corrosion. Therefore, an in-depth understanding of the physicochemical processes taking place in the interior is useful to improve the structure and the performance of the fuel cells.

For this purpose, following experimental investigations and mathematical simulation...
were carried out:

- Experimental measurement of permeability, flow resistance and diffusivity in the porous media
- Modelling of gas permeability and gas diffusion in the porous media
- Laminar and turbulent flow simulation, because the fuel cell may be partly or wholly turbulent
- Analysis of 3-D flow distribution for the given gas channel geometry; it leads to process optimisation which ensures homogeneous fuel gas and air supply for the electrochemical reactions
- Identification of possible structure which causes critical pressure drop

**MATHEMATICAL MODEL**

A mathematical 3-D model was constructed to simulate the flow field distributions. The transport processes in the gas phase are modelled by the Navier-Stokes equation using a detailed transport model including thermal diffusion. For the flow calculation, the mass source term and external body forces like buoyant forces are neglected, thus the conservation equations are:

Continuity equation:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \vec{v})}{\partial x_j} = 0
\]  

Species conservation equation:

\[
\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i \vec{v})}{\partial x_j} + \frac{\partial (\vec{j}_i)}{\partial x_j} = 0
\]

The diffusion mass flux is introduced as sum of Fick's \( \vec{j}_i^m \) and thermal diffusion \( \vec{j}_i^T \):

\[
\vec{j}_i = \vec{j}_i^m + \vec{j}_i^T = -\rho D_i^m \frac{\partial \rho_i}{\partial x_j} - \frac{D_i^T}{T} \frac{\partial T}{\partial x_j}
\]

where \( D_i^m \) is calculated using multi-component model, \( D_i^m \) and \( D_i^T \) can be taken from the molecular gas theory (4).

Momentum conservation equation in the gas phase:

\[
\frac{\partial \rho \vec{u}_i}{\partial t} + \frac{\partial (\rho \vec{u}_i \vec{u}_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}
\]
with the stress:

\[ \tau_{ij} = \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \frac{2}{3} \mu \frac{\partial u_i}{\partial x_i} \delta_{ij} \]  

[5]

In contrast to the well known transport models in the gas phase, the modelling of processes like diffusion and permeation of gas species in porous functional layers is most challenging, since most transport and reaction limiting steps take place in these layers, but the experimental characterisation in these regions is still very difficult due to the complex porous microstructure. At the start of investigations, the porous structure is assumed to be homogeneous in this paper, so that a global quantity can be used for the considered porous region. A diffusion model consisting of gas phase and Knudsen diffusion is followed

\[ \frac{1}{D_{eff}} = \frac{1}{D_{p}^n} + \frac{1}{D_k} \]  

[6]

A more detailed model will be developed in future.

The gas permeation is described by Darcy law, which gives the superficial velocity in terms of pressure gradient:

\[ \frac{\partial P}{\partial x_j} = -K_j \cdot u_j \]  

[7]

The permeability \( K_j \) is not constant (as discussed later) and therefore is assumed to be a function of the superficial velocity magnitude \( |\vec{u}| \) of the form (5):

\[ K_j = \alpha_i \cdot |\vec{u}| + \beta_i \]  

[8]

The mathematical models are solved with CFD program Star CCM+, which applies the method of Finite-Volume to solve the differential equation system. In order to simplify the numerical treatment a single planar solid oxide fuel cell has been investigated and the grid system was generated by ICEM CFD.

Numerical calculations have been implemented using the laminar and different turbulence models in stationary mode. The low Reynolds number k-\( \varepsilon \)-model is assumed to meet the wall boundary condition the nearest. The high Reynolds number k-\( \varepsilon \)-model in combination with the wall function model, and a modified version of it, the Chen's k-\( \varepsilon \)-model were also tested but gave no significant changes of the flow field. For details about the turbulence models, see (5).

For the inflow conditions on the air and the fuel gas sides, inlet velocities were set so that the required mass flow rates were reached. To ensure an even gas distribution at the active surface, velocity profile can be varied at the air and fuel inlets. For the outflows, the pressure outlet setting with a pressure difference of zero was chosen to record a
possible backflow. The input values for the porous media calculation were the diffusion coefficients of the gas components, the permeability of the form shown in equation [8] and the porosity, which is implemented by multiplying with the fluid density in the time derivative terms of the continuity, energy and species equations.

EXPERIMENTAL INVESTIGATIONS

The transport relevant coefficients were determined experimentally under as close to operating conditions as possible; the method and the arrangement of equipment are discussed below.

Permeability

The gas permeability of porous layers was measured using a test set-up shown in Fig. 1, the samples were put onto a metallic plate which has several inlet and outlet installations and is isolated with a metallic box. To avoid a leakage between the sample and the plate, a weight can be added. The pressure at inlet and outlet was measured with digital multimeter, the volume flux was detected using flow meter. As test gas air was used, but any other gases could be taken into account. The measurements were carried out at room temperature.

Various metallic and ceramic substrates were tested. Two samples are presented in this work, they were made of porous ceramic and taken from the Technetics, Florida as described in (3). One sample had a thickness of 2 mm, the other one was pressed to a thickness of 1 mm.

Figure 1. Schematic illustration of test equipment for the gas permeability measurement.

Figure 2 shows the measured results of pressure gradient as function of volume flux. The points represent experimental data, they are fitted with curves of polynomial. As described in the mathematical modelling, the gas permeation is normally stated in terms of Darcy law (see eq. [7]), which denotes a linear correlation between the driving force and the superficial velocity. Since the pressure drop must be zero for zero velocity, the
data fitting must go through the origin. It is obvious that no line which really fits the data well can be found, so the Darcy law may be invalid in this case. Therefore, a correction term with regard to the dependence of velocity is considered and a polynomial is used.

Based on the parameters determined from the fitting curve, the permeability can be calculated.

Furthermore, the permeability for anode and cathode are determined in a similar way.

![Graph showing pressure gradient as a function of volume flux.]

**Figure 2. Pressure gradient as a function of volume flux.**

**Flow Resistance**

In the thin film concept, metallic substrate plays an important role, two main functions of this component are: to support the vacuum plasma sprayed layer fabrication and to form the gas channels ensuring sufficient gas supply.

From the point of view of gas supply, flow properties like flow resistance provide important information for the operation control and can lead to structural improvement.

Experiments have been performed for relevant operation conditions. The metallic substrate samples were first housed in a high temperature and oxidation resistant metallic box, the box was connected with a tube and then set up in a furnace. The furnace was heated electrically, the heating rate and thus the temperature profile can be controlled by programming. The air stream was preheated via heat transfer from tube in the furnace. The flux was controlled and measured with a flow meter. The pressure drop was calculated as difference between the pressure measured at the inlet and in environment.

Fig. 3 shows the experimental data of one metallic substrate used in fuel cell at temperatures of 600°C and 800°C, respectively. The flux was varied in a wide range. It can be seen that the pressure drop is proportional to the flux at both temperatures.
Figure 3. Flow resistances of a tested metallic substrate at temperatures of 600°C and 800°C, respectively.

Porosity

The porosity of the porous substrates and the electrodes was determined using mercury porosimetry. For validation, polished specimens were prepared and microscopically analysed. The colour image of the polished section was then modified to grey scale. Using a special analysis software, the regions of particles and empty space were digitally separated into white and black zones (see images in Fig. 4), the areas of all white and black zones were counted and the porosity determined by evaluating the area quotient. Note that the results from the two methods may not be in agreement, because the porosimetry method gives open porosity, while the image analysis of polished section yields the total porosity.

Figure 4. Polished microscopical image of a Technetics substrate (left) and its re-treated, digitised image (right). The porosity was determined to be 61%.

Diffusivity

The effective diffusion coefficients in ceramic layers were determined using the Wicke-Kallenbach-method, the results will be presented elsewhere.

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RESULTS AND DISCUSSION

The numerical calculations were performed with Star CD using the laminar and turbulent models. The air and fuel flows were treated separately using a counter flow configuration. The required parameters for the setup of the porous media model were taken from experimental data.

Air Flow

The laminar flow on the air side (see Fig. 5) shows the desired even distribution in all channels with a velocity of about 5 m/s. The rapid streams at both edges result from a not-completely closed bypass, but the amount of bypassing air remains small.

![Figure 5. Velocity profile of laminar air flow.](image)

The turbulent flow condition (Fig. 6) shows also a uniform air distribution of a slightly higher velocity than with the laminar model.

Fuel Flow

On the fuel side, the laminar flow setting (Fig. 7) also shows the desired spreading in the region of the active surface with a velocity of about 0.15 m/s.

As could be seen in Fig. 8, the turbulent condition results on the fuel side in a slightly slower velocity than the laminar conditions, in contrast to the air side. This could be an effect caused by the rough surface of the porous media resulting in enhanced turbulence dissipation.

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Figure 6. Velocity profile of turbulent air flow.

Figure 7. Velocity profile of laminar fuel flow.
The flow in the porous anode substrate and the support layer shows an even distribution with only small velocity components in orthogonal directions to the flow (see Fig. 9). This is due to the lack of any driving force in these directions because of the fact that no chemical reaction schemes have been taken into account.

Simulations using the turbulent models (Fig. 10) show no appreciable differences to the laminar one.

Figure 8. Velocity profile of turbulent fuel flow.

Figure 9. Laminar velocity profile in porous substrate and support layer.
Pressure Loss

The pressure drop across the porous media corresponds to the measured results shown in Fig. 3. This verifies the measured diffusion coefficients and the permeability coefficients.

CONCLUSIONS

The porous media in solid oxide fuel cells as the region of highest interest relating to the cell performance has been characterised by the introduced measurement methods. As a control, three-dimensional CFD-analysis shows realistic flow fields, and the resulting pressure drops are in accordance with the corresponding measurements under operating conditions. The influence of diffusivity on local gas concentrations in porous layers, heat transfer and voltage-current distribution will be presented in future works.

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