MODEL CALCULATION OF THE PLANAR SOFC BY THE FINITE VOLUME ELEMENT METHOD

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ABSTRACT

Using the fundamental laws of energy, mass and charge conservation, the temperature, concentration and potential fields of the planar SOFC are calculated by the FIT (Finite Integral Technique). This calculation takes into consideration the diffusion of gases in the porous electrodes, the nonlinearity of the electrochemical reaction and the cermet structure of the anode. The computational method applied offers the opportunity of obtaining a fine local resolution by using the multigrid technique.

1. INTRODUCTION

The solid oxide fuel cell (SOFC) could have an important role in the future as an energy converting system. In the cell, the fuel gas and the oxidant are reacted electrochemically to generate electricity from the free energy change of the cell reaction.

At the cathode

\[
\frac{1}{2} O_2 + 2 e^- \leftrightarrow O^{2-}
\]

At the anode

\[
H_2 + O^{2-} \leftrightarrow H_2O + 2 e^-
\]

Thus the overall reaction is

\[
H_2 + \frac{1}{2} O_2 \leftrightarrow H_2O
\]

The methane reforming reaction could also be taken into consideration. In order to operate the cell at high efficiency, it is important to know the temperature, potential and concentration distribution in the cell to determine operation conditions. The aim of this calculation is optimization of the planar SOFC with hydrogen or reforming gas as the fuel with a precise consideration of the structure and processes at the electrodes.

2. THEORY

The mathematical formulation is based on the conservation laws for mass, charge and energy. For each of these quantities the flux out of a given volume V equals the sources in that volume. The corresponding expression is given by the Gaussian formula (a), where \( d\sigma \) and \( dV \) are area and volume elements, \( Q \) is the source density.
\[
\iint_{\partial V} \mathbf{F}_n \, ds = \iiint_V \nabla \cdot \mathbf{Q} \, dv
\]

(a)

and \( \mathbf{F}_n \) is the flux in the direction of the outer normal.

Further equations tie the flux to the corresponding scalar quantity (b):

\[
\int_x^y (\mathbf{p} \cdot \mathbf{I}, \, ds) = U(x) - U(y)
\]

(b)

For the electric current it is the electric voltage \( U \), for the heat flux the temperature \( T \) and for the mass flux the stream potential \( S \). The electric potential for lines not crossing the electrochemical reaction surface is given by the line integral between the two corresponding points where \( \rho \) is the local resistivity and \( ds \) the line element.

The potential difference between the points crossing the electrochemical reaction surface is given by the sum of nonlinear dependency analogous to the Butler-Volmer equation (c) and the ohmic part.

\[
I_n = I_0 \sinh (\gamma (\Delta U - \Delta U_0) \frac{F}{RT}) \quad \text{with} \quad \Delta U = \lim_{x \to y} U(x) - U(y)
\]

(c)

The constants \( \gamma \), \( \Delta U_0 \) and \( I_0 \) depend on the electrochemical process involved, as well as on the materials and geometry used. Boundary conditions are given either by the voltage \( U \) or by the current density \( I_n \).

The heat flux consists of a diffusive and a convective contribution. The diffusion flux is treated similarly to the electric current, the convective heat flux depends on the mass flux vector. Heat sources are both the ohmic losses and the electrochemical reaction, which consists of an entropy and an overvoltage term. The stream potential \( S \) is a mathematical quantity with no obvious physical interpretation, the definition of which is analogous to the definition of the temperature \( T \) and electric voltage \( U \).

### 3. COMPUTATION TECHNIQUE

The volume of the SOFC is discretised by the finite integral technique (FIT)(1), and the balance equations for the flows \( F \) (current, heat, mass) at each discrete volume point \( X \) is equal to the sources in the volume (Fig.1).

\[
F_r + F_i + F_u + F_o + F_v + F_h = \text{sources in the volume}
\]

(d)

This equation is transformed for each point \( X_m \) to achieve the final form of the equation.
for the calculation:
\[ a_Y Y_r + a_Y Y_1 + a_Y Y_u + a_Y Y_v + a_Y Y_h + a_Y Y_m = \text{sources} \quad (e) \]

with \( a_Y = \) conductivity in i-direction, \( Y_i = \) field value at point \( X_i \)

For the modelling we assume the following situation:
There is only conductive transport in the gas channels and diffusion of the gases in the porous electrodes. We have adiabatic boundary conditions in two directions and periodic conditions for the temperature in the direction of the stack. Between the bipolar plates a constant potential difference is assumed, which matches the operating voltage of the cell. The potential jump at the electrodes is modelled by a double layer of charges and surface resistivity (2).

The resulting equation systems are solved by a multigrid algorithm (3). As a result, the local potential, temperature and concentration distributions in the cell are obtained in all three directions in space.

The raw data for the calculation are the geometrical dimensions and the operating data of the cell, as well as the conductivity of the materials. The thermodynamic and fluidic data for the calculation of the temperature and concentration are known from the literature (4,5). The data necessary to determine the potential field were obtained experimentally from impedance and polarization measurements. The information on the electrode kinetics obtained in this way may be used directly for a 3-dimensional calculation of the SOFC electrode reaction. The potential field is coupled to the temperature and concentration via the Nernst and Butler-Volmer equations. There is a feedback from the temperature to the voltage from the ohmic losses in all regions of the cell and from the polarization heat at the electrodes. The concentration is coupled to the potential in the electrodes via Faraday's law. These relationships require an iterative calculation of the individual systems.

For the computation of the influence of the anodic cermet structure and of the influence of the supports and gas channels the following parameters were used:
- exchange current density \( i_o = 0.1 \text{ A/cm}^2 \) (Fig.2), \( i_o = 1.0 \text{ A/cm}^2 \) (Fig.3)
- input temperature \( T_i = 1073\text{K} \)
- hydrogen velocity \( v_{H_2} = 1\text{cm/s} \)
- oxygen velocity \( v_{O_2} = 10\text{cm/s} \)
- oxygen partial pressure \( P_{O_2} = 0.2\text{bar} \)
- hydrogen partial pressure \( P_{H_2} = 0.9\text{bar} \)

4. RESULTS

Since the computation technique applied enables a separate calculation of the individual potential positions, both of the metal and also of the electrolyte in the same anode volume, it was possible for the first time to model the influence of the cermet structure
of the anode on the curve of the characteristic.  
As examples, Fig. 2 shows the way in which the current density/voltage curves of an SOFC are influenced by taking the fine structure of the anode into consideration. A slight improvement in the cell characteristics can be observed which, in the case of an output voltage of 0.7V, amounts to about 10%.

As a further example, Fig. 3 shows the current density distribution in the electrolyte vertical to the direction of gas flows in a 5 x 10 cm cell with 5 gas channels. The maximum current density is observed at the fuel inlet and decreases in the direction of the fuel flow. It is apparent that the current densities below the gas channels are lower than below the supports.

Fig. 4 shows the local current density/voltage curve along the gas channel in co-flow operation of the cell. The maximum current density is observed in the middle of the cell at low output voltage (U < 0.6 V) and at the gas outlet at high cell operating voltage (U > 0.6 V). At the gas inlet the cell characteristic has linear behaviour and further on it increases to higher current densities at low output voltages due to heating of the cell. Finally the fuel consumption causes a drop in the curves at low operating voltages. This figure demonstrates the influence of the temperature as well as the concentration of the gases on the current density/voltage curves of the cell. Fig. 5 shows the same cell in counter-flow operation (Fuel in -Z direction). It is apparent that the maximum current density is present at the fuel inlet and drops rapidly along the direction of fuel flow. At the air inlet linear behaviour is observed. This figure indicates a higher current density of counter-flow operation in comparison to co-flow operation, but also a heterogeneous current distribution across the cell layer. The linear characteristic at the air inlet under both operating conditions shows that the air flow dominates the temperature in the cell.

5. CONCLUSIONS

The computational method applied enables very fine 3D-local resolution of the electrode structure using the multigrid technique. The separate calculation of the individual potentials both of the metal and of the electrolyte in the same volume of the anode is possible. For this reason, the method possesses the ability to give a description of the pore structure and to formulate expressions for the mixed conductivity in the system. The application to problems of electrochemical kinetics with a simultaneous consideration of the electrode geometry can be implemented. This enables a detailed description of the actual working conditions in the SOFC and a very effective process modelling.

6. REFERENCES

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Fig. 1. Schematic model of the calculation method
Fig. 2. Influence of the cermet structure of the anode on the characteristic curve of the cell in co-flow operation.

Fig. 3. Influence of the supports and gas channels on the current density distribution in the electrolyte.
Fig. 4. Local current density/ voltage curve in the direction of the gas flow, co-flow operation, gases in Z direction.

Fig. 5. Local current density/ voltage curve in the direction of gas flow, counter-flow operation, hydrogen in -Z direction.