THE DEVELOPMENT OF HEAT TRANSFER AND GAS FLOW MODELING IN THE SOLID OXIDE FUEL CELLS (SOFCs)

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ABSTRACT

There are sources of heat generation and absorption in SOFCs, which are affected by gas parameters in the fuel cells. These sources cause heat transfer to the flowing gases. The pressure drop caused by flow resistance in the channels has effects on the distribution of temperature and gas flow rate. Some modeling work has been carried out under the assumption of laminar flow during the last few years. The present work concerns a review of heat transfer and gas flow modeling developments in the SOFCs as well as some new modeling development. The different models are compared in terms of model level (unit or stack, system), flow type (cross-, co- or counter-flow) and developed or developing flow, thermal source considered, boundaries used in the model, models of heat transfer to the gas and whether the pressure drops were considered in the model. Some useful remarks and conclusions are drawn. Results from a new modeling approach are also provided.

INTRODUCTION

Fuel cells continuously convert chemical energy into electrical energy through electrochemical reactions at the anode and cathode. Among these, high temperature fuel cells are of particular interest. This is because operation at high temperatures allows for the use of natural gas as a fuel, and allows hybrid concepts involving a combination of fuel cells and a gas turbine. The overall system efficiency can be significantly increased.

Operation at a temperature about 1000 °C and pressure greater than one atmosphere leads to solid oxide fuel cells (SOFCs) as the obvious choice (1). SOFCs differ from other fuel cell technology in that the electrolyte is solid. There is no consumption of the electrolyte eliminating the need for electrolyte replenishment and there is no corrosive liquid. SOFCs also improve reliability since they can be built without any moving parts (2).

Different coefficients of thermal expansion, interdiffusion of materials used for the anode, electrode and cathode, and stresses caused by temperature gradients are the major engineering problems faced in the design of SOFCs (3). To deal with the problem of the selection of stable, durable materials, the modelling of heat and mass transfer in SOFCs is crucial and important to the successful design and operation of SOFC system.
During recent years, a number of mathematical modeling works have been presented to simulate the heat transfer and gas flow in SOFCs (3-8). The most research works are based on some assumed heat transfer conditions and certain simplifications, like constant solid temperature, fully developed laminar flow in the manifold and/or cell channels. Through a literature survey, the present paper summarizes the published developments and state-of-the-art of heat and mass transfer modeling in SOFCs. In addition, a new approach is presented and some new results are given.

BACKGROUND

There are different kinds of SOFCs structure, namely tubular, planar, and monolithic design. The different designs differ in flow paths, internal cell resistance losses, and in the cell-to-cell electrical connections (interconnectors). But the main components in SOFCs are common, namely positive electrode (anode), electrolyte and negative electrode (cathode), abbreviated as PEN hereafter, and interconnector between PENs.

![Figure 1. Fuel Cell Stack with Manifolds.](image)

![Figure 2. Fuel Cell Stack Geometry.](image)

The number of PEN in a stack may be as many as hundreds, which may be mounted one upon the other and electrically connected by interconnector into a stack. The reactants are fed to and discharged from each of the cells through feed and exhaust...
manifolds. Figure 1, from (2), is a monolith fuel cell stack with inlet and outlet manifolds, and Figure 2 shows a stack geometry with channels, see (3).

As mentioned above, SOFCs operate at high temperatures (about 1000°C), as there are four heat sources in the fuel cells. Two of the source terms produce heat (Qel and Qohm) and the other two absorb heat (Qref and Qshd). The source term can be written as

\[ Q = Q_{el} + Q_{ohm} - Q_{ref} - Q_{shd} \]  

\[ Q_{el} = \frac{m_{a} T_{i}}{5} (\frac{\Delta S}{\Delta T}) \]  

\[ Q_{ohm} = \frac{m_{f} T_{i}}{5} (\frac{\Delta S}{\Delta T}) \]

where \( m_{a} \) and \( m_{f} \) are flow rates of air and fuel, respectively, \( \Delta S \) are entropies of the components, \( \Delta S_{o^{2}i} \) is the transported entropy of the oxygen ion, and \( \Delta S_{e^{*}} \), the transported entropy of the electrons.

- Electrochemical heat generation (Qel) includes heat generated by electrochemical reaction at the electrode-electrolyte interface and by the diffusion of the reactants in the porous anode and cathode. It can be written as \( Q_{el} = Q_{cat} + Q_{anh} \) in which (7)

\[ Q_{cat} = T_{cat} (\frac{\Delta S}{\Delta T}) \]  

\[ Q_{anh} = m_{f} T_{i} (\frac{\Delta S}{\Delta T}) \]

- Ohmic heat (Qohm) is caused by the electrical resistance to current flow. It is generated throughout the solid structure since electrical current flows in this region. The two regions dominating this heat are the interconnect and electrolyte. It is written as \( Q_{ohm} = I^{2}R \).

- Heat reforming (Qref) and shifting (Qshd) are related to the reactions when the methane or natural gas is used as fuel. Both of them absorb heat.

The inlet temperature of gas flow is about 400 °C (without pre-heating process) or 650 °C (with preheating process) (1). Heat transfer occurs in the following ways:

- between cell component layers and flowing air and fuel streams. This can be described by forced convective heat transfer with or without natural convective heat transfer in terms of heat transfer coefficients \( \alpha_{a} \) or Nu.

- between the fuel and air streams across the interconnect layer in terms of the overall heat transfer coefficient, U.

- in solid structures in terms of heat conduction with different thermal conductivities, \( \lambda_{i} \) (i = cathode, anode, electrolyte and interconnect layer).

Due to the flow resistance in the fuel cells, pressure drop (ΔP) along the channel and manifold can cause non-uniform distribution of flow rate and temperature, and different output of electrical energy in terms of voltage potential (5) and even gas recirculation. Under some severe conditions, the lack of gas in some channels can cause irreversible damage to the fuel cell components. Pressure drop depends on the channel and manifold structures, flow streams etc.
PROBLEM STATEMENT

Despite similarities in geometry, the problem analyzed here is fundamentally different from that of heat exchangers or catalytic reactors in that the solid acts as the electrolyte across which oxygen ion transport occurs. As discussed above, electrochemical heat generation $Q_{ei}$ is related to entropy changes and transported entropies in the cell, since the oxygen ($O_2$) in the cathode is changed into oxygen ion ($O_2^-$) and finally into $H_2O$ in the anode. The partial pressure of species in the channels thus varies and affects the heat transfer and pressure drops. The heat transfer, gas flow and electrochemical reactions are coupled with each other. This introduces an integral electron conservation balance which results in an integro-differential problem.

The physical processes taking place in the SOFCs are highly complex, and there are still uncertainties related to the heat transfer and gas flow, and also the limitation of computer resources. To get meaningful results and physical insight into the complex but interesting processes, some assumptions in the modeling are necessary. The following are possible items, which should be considered when a simulation is to be performed:

- Heat source terms, which include the amount of heat generated, their distribution and relationship with other parameters.
- Heat transfer model in the solid structures, and between solid surfaces and flowing gases. The gas flows may be considered steady or time dependent, one-, two- or three-dimensional, forced convection heat transfer with/without natural and radiative heat transfer, with uniform, constant or other kinds of boundary conditions, etc.
- Fully developed or developing laminar or turbulent flows in all flowing gas channels and manifolds.

THE DEVELOPMENT OF THE MODELING

During the last few years, considerable attention has been paid to the modeling of SOFCs. Attempts to simulate the velocities, pressures, temperatures, mass fractions, electric currents and potentials in SOFCs under certain boundary conditions have been presented. To gain an insight of the knowledge in this area, a brief summary of the literature is presented. The survey only covers literature dealing with the relevant problems of heat transfer and gas flow modeling.

Vayenas (1985) created a two-dimensional mixing cell model for cross-flow to simulate the distribution of gas species, temperature, and current density. The schematic diagram employed is presented in Figure 3. The five unit batteries were connected in series and each consisted of 100 channels electrically connected in parallel. For modeling purpose, the unit battery was considered to be composed of $K \times L$ unit cells, which are shown in Figure 4. It was assumed that the temperature for both solid and gas streams, and gas-phase composition were uniform. For the gas streams, the convective heat transfer coefficient was given by

$$\alpha_t = \alpha_s = 0.253[(b_1+c_1) / 2b_1c_1] \text{ W/m}^2\text{K}$$  \[4\]
In this expression, $b_1c_1$ are geometry parameters of the unit cell. To account for the effects from the outer cell layers, the perfect thermal insulation at the outer unit cell walls was used to simulate adiabatic behavior.

Figure 3. Schematic Diagram Employed by (6).

Figure 4. Unit Cell Geometry (6).

Figure 5. Cell Layers Within Cross-flow of SOFC (4).

Another model was developed by Ahmed et al. (1991) (4). This could be used to simulate the electrochemistry and thermal hydraulics in a cross-flow monolithic solid oxide fuel cell with alternating layers of anode, electrolyte, cathode, and interconnect. Dividing a unit cell into a number of nodes, the model sets up the steady-state heat and mass transfer equations for each node in a cell layer. The heat source in the node is from the resistance to current flow and from the entropy change of the electrochemical reaction. Based on the average thermal and compositional conditions, Nusselt number value of 3.0 and the equivalent diameter of rectangular flow channels were used for convective heat transfer between gases and the solid surface. The heat transferred between the fuel and air streams across the interconnect layers was also considered by the
overall heat transfer coefficient, $U$. In this model, the generated heat was regarded to be released in the electrolyte, and constant resistance was used for all layers except for the electrolyte layer. As assumed with the fully developed laminar flow, the frictional pressure drop in the channels was expressed in the form:

$$\Delta P = \frac{(\mu u KL)}{(ab^3 \rho c)}$$  \[5\]

**Ferguson et al. (1996) (3)** proposed a three-dimensional mathematical model of a solid oxide fuel cell, which allows the computation of the local distribution of the electrical potential, temperature, and concentration of the chemical species. It was claimed that the heat generated by internal resistance was very important. In the gas channels, the thermal flux is mainly convective in the gas flow direction and conductive from the channel to the solid part:

$$q = \sum_{i \in G} C_{\text{pi}} N_i - \lambda \text{grad} T$$  \[6\]

Here $G$ is the set of various components of the gas mixtures, $\lambda$ is the thermal conductivity. In the solid parts, the thermal flux is mainly conductive and modeled by Fourier's law of heat conduction. The volume heat source term, $Q$, is modeled as the ohmic heat source, and shifting, reforming reaction sources plus the heat generated by the electrochemical reaction. The boundary conditions considered are based on the idea that the cell is part of a whole stack and that the overall behavior is periodic. Periodicity conditions are imposed for the temperature on the top and bottom boundaries $\Gamma_T$ and $\Gamma_B$ of the cell ($T_{r_T} = T_{r_B}$), while insulation conditions were imposed on the lateral boundaries $\Gamma_L$ ($T_{r_L} = 0$).

A computer code, namely KAMELEON SOFCSIM, was developed by **Melhus and Ratkje (1996) (7)**, and used to find simultaneous solutions of all conservation equations for mass, energy and momentum in a quasi three dimensional (two space dimensions, $x$ and $y$, plus time variation), for single, flat SOFCs. The reduction of the mass of $O_2$ in the cathode chamber, consumed in the reaction with fuel, was assumed to be regained in the anode as $H_2O$ for the mass balance. The heat sources were connected with the entropy change and transported entropy, plus the reaction overpotentials. The sink and source terms of heat were evenly distributed in the control volumes of the electrode. In this investigation, adiabatic surfaces were chosen for the solid materials. Both gas flows were in developing laminar flow. The maximum velocity is not in the center of the channel, but shifted away from the electrodes. It is typical for a diffusion controlled reaction claimed by the authors. The pressure drop was 3 Pa along the fuel channel, and 0.3 Pa along the air channel. The temperature rises about 200 °C along 5 cm for an initial air velocity of 25 cm/s.

Regarding the distribution of gas flow, **Boersma (1997) (8)** developed a model that can simulate the non-uniform gas flow distribution along the height of a fuel cell system. Some of the resistances are constant, while some depend upon the gas velocity. The most important pressure drop was caused by the channels adjacent to the active cell area, which was inferred from laminar flow formulae in this model. The pressure drop was
\[ \Delta P_c = K_c \Phi \quad \text{with} \quad K_c = \left( \frac{f \eta l_c}{kA_cD_{hc}^2} \right) \]  

where \( \Delta P_c \) is the total pressure drop in the channel, \( \eta \) is the gas viscosity, \( k \) is the number of channels in the plane parallel to be allocated to one manifold channel, \( l_c \) is the corrugation length, \( A_c \) is the cross sectional area of one corrugation, \( D_{hc} \) is the hydraulic diameter of one corrugation, \( \Phi \) is the flow that passes the cell area considered, and \( f \) is a friction factor that depends on the channel geometry. The resistances caused by the flow through the manifold channels were considered by splitting the flow in the inlet manifold channels and combining it with the flow in the outlet manifold channels. They were simulated by

\[ \Delta P_{mi} = K_1 \Phi_i^2 \]  
\[ \Delta P_{mo} = K_2 \Phi_o^2 \]  

where \( \Phi_i, \Phi_o \) are the flows in the inlet and outlet manifolds, respectively. \( K_1 \) is the sum of resistances of the rough pipe flow and the resistance due to splitting and \( K_2 \) represents the sum of the resistance of the rough flow and the resistance due to combining.

**REMARKS**

Table I shows the comparison of heat transfer and gas flow modeling works for the SOFCs discussed above.

**Table I. Comparison of Heat Transfer and Gas Flow Modeling Works for SOFCs**

| Authors            | Vayenas et al. (1985) | Ahmed et al. (1991) | Ferguson et al. (1996) | Melhus et al. (1996) | Boersma (1997) |
|--------------------|-----------------------|---------------------|------------------------|----------------------|----------------|
| Model level        | Unit and stack        | Sub-unit (node)     | Unit                   | Unit and channels    | Channels and stack |
| Flow Type          | Cross-                | Cross-              | Co-                    | Co-                  | Count- in manifolds |
| Thermal source     | No                    | Entropy change, Resistance | With shifting and reforming | Entropy change, Resistance | No |
| Boundary conditions| Uniform temperature   | Periodic, Isolated | Adiabatic              | No                   |
| Thermal model      | Convection            | Convection, Combined heat transfer | Convection, Conduction | Convection, Conduction, Mass | No |
| Flow model         | Fully developed       | Developing laminar  | Laminar                |                      |
| Heat transfer      | \((\alpha_s = \alpha_m = 0.253(b_1 + c_1)/(2b_1c_1))\) | 3.0                  | Not clear              | Not clear            | No |
| Pressure drop      | No                    | Yes                 | No                     | Yes                  | Yes |

It is obvious that there are some limitations in the models proposed by different authors, either in assumptions regarding the thermal sources and boundary conditions, or simplified thermal models. The temperature, velocity and pressure drop were simulated

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by the assumption of laminar flow in all the models discussed above. It is also the fact that in these models the heat transfer coefficients $\alpha_a$, $\alpha_v$ or Nusselt numbers $Nu$ were assumed known. Papers considering prediction of the thermal problems and gas flow problems coupled with the electrochemical reaction in the fuel cell to get the true heat transfer coefficients are rare.

**NEW MODELING APPROACH**

A new modeling approach has now been applied to simulate a single cell channel with rectangular cross section (Figure 2). Figure 6 shows the cross section of the channel with dimensions of $b_1$ and $c_1$. The lower surface of the channel is connected to the electrode layer. One purpose is to achieve more realistic wall boundary conditions than previously investigated.

As discussed above, the heat generated by the electrochemical reaction at the interface of electrode and electrolyte, together with the heat caused by the electrical resistance to current flow in the solid structure, is conducted to the flowing gas. The diffusion of the reactants in the porous anode and cathode causes mass transfer and also heat in the electrodes. Thus the gas flow is affected.

In this approach, heat sources, convective heat transfer between the channel surface and flowing gas are considered. For simplicity, the gas flows in a straight cell channel. Fully developed laminar flow is considered. The boundary conditions are:

- Constant heat flux $q$ at one surface which is adjacent to the electrode/electrolyte layer.
- Constant temperature $T$ at the other three surfaces.

The finite volume computer code SIMPLE HT (10) is used in this work. The code is generally designed for the solution of the steady two-dimensional, laminar and turbulent convective heat transfer and fluid flow problems. The pressure-velocity coupling is treated by the SIMPLE, SIMPLEXC or SIMPLEX procedures with the incompressible form of the pressure-correction equation. The convection-diffusion may be treated by the power-law, upwind, hybrid or central difference schemes.

This code was used here to simulate a single unit cell channel for different $b_1/c_1$ ratios. Some results are presented in Table II. Table III shows the comparison with other results from the literature. In Table II and III, $b_1$, $c_1$ are geometry parameters of the rectangular channel, $C$ is the pressure drop factor ($f = C/Re$), $\lambda$ is the thermal conductivity of the flowing gas.
Table II. The New Approach Results.

| $b_l/c_l$ | 1:1 | 2:1 | 3:1 | 5:1 | 7:1 | 10:1 |
|-----------|-----|-----|-----|-----|-----|------|
| C         | 56.26 | 61.33 | 67.49 | 75.28 | 79.67 | 83.44 |
| Nu        | 3.53 | 3.84 | 4.49 | 5.50 | 6.12 | 6.68 |

Table III. The Comparision of Nu Results.

| $b_l/c_l$ | Veyenas model (1985) | Ahmed model (1991) | New approach |
|-----------|----------------------|-------------------|--------------|
| 1:1       | 0.253 $\lambda^{-1}$ | 3.0               | 3.53         |
| 3:1       | 0.253 $\lambda^{-1}$ | 3.0               | 4.49         |
| 10:1      | 0.253 $\lambda^{-1}$ | 3.0               | 6.68         |

It is clear that there is a relationship between the pressure drop, heat transfer and geometry parameters. The Nu number is sensitive to the wall boundary conditions and it is believed that the new approach is more accurate.

If the mass transfer through the wall is considered, both the heat transfer and the pressure drop (friction factor) will be affected. However, the results of such an investigation will be the subject of another paper.

CONCLUSIONS

If the electrochemical reaction by oxygen ion transport through electrolyte is taken into account, the heat transfer and gas flow analysis in SOFCs becomes very complicated. There are still many uncertainties involved in such analyses.

The present work reviewed published papers on heat transfer and gas flow modeling for SOFCs. Through the description of the different models and comparison between them, it was found that almost all of the works were based on laminar gas flow with certain constant heat transfer coefficients or Nusselt numbers.

A new modeling approach was presented and some results were given. The importance of real thermal boundary conditions was revealed.

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