MODEL CALCULATION FOR PLANAR SOFC
FOCUSED ON INTERNAL STRESSES

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ABSTRACT

The concentrations of the chemical species, the temperature
distribution, the potential distribution, and the current density
in a planar SOFC were calculated using a single-unit model
with double channels of co-flow or counter-flow pattern. The
finite volume method was employed for the calculation, which
is based on the fundamental conservation laws of mass, energy,
and electrical charge. The model was constructed in detail to
include the internal- or external steam reforming, the water-
shift reaction, and the diffusion of gases in the porous
electrodes. The effects of the cell size, the operating voltage
and the thermal conductivity of the cell components on the
calculated results were investigated. From the simulated
temperature distributions in the electrolyte and the
interconnector, the stress distributions were calculated using
the finite element method. The results demonstrated that the
steam reforming would generate internal stresses of several
tens MPa in an electrolyte.

INTRODUCTION

The solid oxide fuel cells (SOFCs) are promising candidates for future
energy conversion systems because of their higher energy conversion
efficiency than those for conventional heat engine systems and other types of
fuel cells. In addition, internal reforming of natural gas can be performed
at the anode, which allows direct use of natural gas as the fuel.

In SOFC stack designs, the planar type design has received much attention
recently, because it is simpler to fabricate and easier to be made into various
shapes than the other type designs. Besides, the planar type SOFC offers
higher power density relative to the tubular type SOFC, which is ascribed to
the low electrical resistance due to shorter current paths. However, the
status of the development is still at a module level, and some technical issues
have not been solved yet. The internal stresses in cell components arising
from thermal shocks or heat cycles are one of the problems to be solved.
The planar type SOFC requires high-temperature gas seals at the edges or
around the internal gas manifolds. For this purpose, cement, glass, and
glass-ceramic seals are expected to give sufficient sealing efficiency. However, the strict binding among each cell component generates mechanical constraints, and thus a slight mismatch in thermal expansion coefficient (TEC) among the cell components can cause a large stress. Moreover, because of non-homogeneous temperature distributions inside the cell, cell components are irregularly deformed, adding a large internal stress. As a consequence, the thermal expansion coefficient matching among the cell components and mitigation of the non-homogeneous temperature distributions in the cell components are indispensable to reduce the internal stress. Some parameters of stack design and operating conditions, such as cell geometry, internal or external steam reforming, thermal conductivity of the components, and cell operating voltage affect the temperature distributions inside the cells in a complicated way, and thus it is difficult to optimize these parameters independently to lower the internal stresses. The computer simulation technique has been used to investigate the cell performance in SOFCs, and considered to be an effective way to analyze the effects of these parameters on the temperature distributions inside the cells (1-8). The purpose of the present work is to estimate the tensile stresses in the cell components using a three-dimensional model simulation. In order to derive the stresses, we calculated the temperature distributions in the cell components in the first step. We employed simplified single-unit models with co-flow or counter-flow bipolar channels, and calculated the concentrations of the chemical species, the potential distribution, the local and average current density, and the temperature distribution inside the cell. The simulation model was constructed in detail to include the internal- or external steam-reforming, the water-shift reaction, and the diffusion of the gaseous species in the porous electrodes. In the second step the tensile stresses in the cell components were computed from the temperature profiles. The internal stresses were estimated as a function of the cell size, the operating voltage, and the thermal conductivity of the cell components, and thus suitable operating conditions to reduce the internal stresses have been proposed.

MATHEMATICAL MODEL

A simplified single-unit cell model with bipolar channels was used for the simulation. The one-cell stack and the single-unit model are illustrated in Fig. 1. For the sake of simplicity in the calculation, we analyzed half of the one repeating unit located in the middle part of the one-cell stack. The thermofluids analysis was performed using the computational fluid dynamics tool “STAR-CD” (Computational Dynamics Ltd.). In STAR-CD, the algebraic finite-volume equations are solved. The solid and fluid parts were divided into small discrete meshes, and in each mesh, the following differential equations governing the conservation of mass, momentum, and energy were solved.

- The mass and momentum conservation (the “Navier Stokes” equations):
The enthalpy conservation equation:

\[
\frac{1}{\sqrt{g}} \frac{\partial}{\partial t} (\sqrt{g} \rho u_j) + \frac{\partial}{\partial x_j} (\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_i} + s_i
\]

[1]

The specific heat of the fluid was treated as the polynomial function of the temperature, while the thermal conductivity of the fluid and the solid, and the specific heat of the solid part were assumed to be independent of the temperature.

For the whole model, the following mass and energy balances should be considered.

• The mass balance of the total gas:

\[
\frac{dM_A}{dt} = M_{in}^A - M_{out}^A + \sum_i S_{i}^A
\]

\[
\frac{dM_F}{dt} = M_{in}^F - M_{out}^F + \sum_i S_{i}^F
\]

[3]

• The enthalpy balance:

\[
\frac{dH_A}{dt} = H_{in}^A - H_{out}^A + Q_A - q_A - q_{EXT}^A
\]

\[
\frac{dH_F}{dt} = H_{in}^F - H_{out}^F + Q_F - q_F - q_{EXT}^F
\]

\[
\frac{dH_S}{dt} = Q_S + q_A + q_F - q_{EXT}^S
\]

[4]

For the thermal boundary conditions on the surface of the solid part, adiabatic boundary conditions at the edges, and cyclic conditions on the surfaces connecting to the next units were employed. For the boundary between the solid and the fluid, the following continuity condition was imposed:

\[
\lambda(x) \nabla T_i(x) \cdot n = \kappa(T_i(x) - T_j(x))
\]

where \( n \) the unit vector normal to the boundary, \( T_i \) and \( T_j \) temperature of the solid and fluid at \( x \) on the boundary, respectively.

The radiative losses were neglected in this model, and thus the whole energy balance equation in the steady state was simplified as follows.
The reactions taken into account are,

(at anode)
steam reforming reaction:

\[
\text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2
\]  

shift reaction:

\[
\text{H}_2\text{O} + \text{CO} \leftrightarrow \text{H}_2 + \text{CO}_2
\]  

electrochemical oxidation:

\[
\text{H}_2 + \text{O}^2- \rightarrow \text{H}_2\text{O} + 2e^-
\]
\[
\text{CO} + \text{O}^2- \rightarrow \text{CO}_2 + 2e^-
\]  

(at cathode)

\[
\frac{1}{2}\text{O}_2 + 2e^- \rightarrow \text{O}^{2-}
\]

Electrochemical reactions were assumed to be instantaneous at both electrodes and occur at the interfaces between electrodes and electrolyte. The shift reaction was supposed to be in chemical equilibrium at any point in the anode.

For the calculation of the electric current, we considered a discrete anode/electrolyte/cathode unit shown in Fig. 2. The direction of the electric current path in the electrolyte was vertical to the interfaces between the electrolyte and electrodes, and the in-plane path was treated as negligible. The electric current \( I_i \) in the \( i \)-th discrete cell was determined by the operating cell voltage \( E_0 \) as follows;

\[
E_0 = E_i - R_i I_i - \eta_i
\]

where \( E_i \) the Nernst potential, \( R_i \) the ohmic resistance, and \( \eta_i \) the overpotential. In the current density range of interest, the diffusion overpotential would be negligible, and thus \( \eta_i \) was assumed to be current-independent. Accordingly using the empirical formula, the sheet resistance \( r_i \) was expressed as follows:

\[
r_i = T /(-434 + 1.25 \times 10^6 \times \exp(-7185 / T)) + 0.04
\]

where the effect of the interconnector geometry was included into the formula as the temperature-independent term.

Supposed that no temperature gradients are present in the discrete anode/electrolyte/cathode unit, the Nernst potential is a function of the
average temperature $T_i$ in the anode/electrolyte/cathode unit and the oxygen partial pressure $P_{O_2}$ at both the electrodes. Accordingly the Nernst potential is given as;

$$E_i = -\frac{\Delta G^0}{12 \times F} - \frac{RT_i}{12 \times F} \ln \frac{P_{CO_i}^2 \times P_{H_2O}^3}{P_{H_2} \times P_{CO} \times P_{CH_4} \times P_{O_2}^3}$$  \[14\]

where $\Delta G^0$ the standard Gibbs free energy change of the electrochemical oxidation of the fuel, $R$ the gas constant, $F$ the Faraday constant, and $P_{CO_2}$, $P_{H_2O}$, $P_{O_2}$, $P_{CO}$, $P_{CH_4}$, $P_{H_2}$ the partial pressures of carbon dioxide, water, oxygen, carbon monoxide, methane, and hydrogen at the electrode, respectively.

The rate of the reforming reaction [7] at the anode can be empirically written,

$$r(1) = k_0 \times \exp\left(-\frac{\Delta E}{RT}\right) \times P_{CH_4}^{AE} \times P_{H_2O}^{BE} \times D_{an}$$  \[15\]

where $\Delta E$ is free energy of activation, $k_0$ is a constant, $P$ is partial pressure, $AE$ and $BE$ are experimental parameters, and $D_{an}$ is the density of the anode. The equilibrium constant for the shift reaction [8] is expressed as,

$$K_{shift} = \exp\left(-\frac{\Delta H_0}{RT} - \frac{\Delta \alpha - \Delta S_0}{R} + \frac{\Delta \alpha \ln T}{2R} + \frac{\Delta \beta T + \Delta \gamma T^2}{6R}\right)$$  \[16\]

where $\Delta H_0$ is the heat of reaction, $\Delta S$ is the change of the entropy, $\alpha$, $\beta$, and $\gamma$ are the coefficients of the temperature-dependent terms in the function for the specific heat.

The reaction rates of the shift reaction [8] are determined for the forward and the backward processes;

$$r(2)_f = k_1 \times P_{CO} \times P_{H_2O}$$

$$r(2)_b = k_1 \times K_{shift} \times P_{CO_2} \times P_{H_2}$$  \[17\][18]

where $k_1$ is a constant.

The electric current density $J$ is expressed by Faraday’s law,

$$J = 4F \frac{dO_2}{dt} = 2F \frac{df}{dt}$$  \[19\]

where $dO_2/dt$ and $df/dt$ are the molar flux rates of oxygen and fuel at the cathode and the anode, respectively. Assuming that hydrogen and carbon...
monoxide are consumed proportionally to the ratio of the partial pressure, the reaction rates are obtained for the reaction [9] and [10].

The diffusion of the gaseous species in the porous electrodes was considered by specifying the molecular diffusivity for each specimen and specifying the momentum source term in a linearized form.

The principal stress in the solid part was calculated from the simulated temperature distribution in the solid part using the finite element program "ABACUS" (Hibbit, Karlsson and Sorensen, Inc.). In the stress calculation, the discrete 3D meshes used for the thermofluid analysis were employed. The operating conditions and parameters are listed in Table 1.

RESULTS AND DISCUSSION

Thermofluid Analysis

We first specified the standard cell operating conditions and parameters for the counter-flow case so that the fuel utilization would be about 80%. With the selected parameters for the operating conditions, the concentrations of the gaseous species, the open circuit voltage (OCV), the distribution of the current density, the average current density, the overall fuel utilization, and the temperature distribution were calculated. Figure 3 shows the calculated concentration profile for CH₄, H₂, and CO at the anode. It can be seen that most of the supplied CH₄ is reformed within the first 10 mm from the fuel inlet, suggesting that the steam reforming reaction is much faster than the electrochemical oxidation of fuel. Consequently, H₂ and CO concentrations rapidly increase within this area, and then gradually decrease as a result of consumption by the electrochemical oxidation while flowing towards the fuel outlet. In the area underneath the interconnector rib, the gaseous species are transported only by diffusion in the porous electrodes. This leads to the lower H₂ and CO concentrations than in the channel area. At the fuel outlet, 80% of the supplied fuel has been consumed, which is consistent with the fuel utilization calculated from the total current.

At just a short distance from the fuel inlet, the temperature of the electrolyte drops rapidly because of the endothermic steam reforming reaction as shown in Fig. 4. In the middle area where the steam reforming reaction is complete, the electrolyte temperature rises because of the exothermic electrochemical reaction. At the downstream of the fuel, the electrolyte temperature decreases along the fuel stream, since the heat generation is small and in addition, the electrolyte is cooled by the incoming air.

Figure 5 indicates the OCV profile. The OCV decreases along the fuel stream, reflecting the decrease of the H₂ and CO concentrations. Since the current density is directly influenced by the values of OCV and R, it first increases, reaches a maximum, and then decreases along the fuel stream as can be seen in Fig. 6. At the fuel inlet, R is large while OCV is high, thus
the value of the current density is not so high. In the middle area where the reforming reaction is complete, both $R$ and OCV decrease along the fuel stream, and as a result, the current density profile shows a peak value of about 0.9 A/cm$^2$. At the fuel downstream, the cell temperature and OCV become lower, accordingly the current density decreases monotonically. Reflecting the lack of H$_2$ and CO, the current density is as low as 0.073 A/cm$^2$ in the area underneath the interconnector rib, and thus the average current density comes down to 0.39 A/cm$^2$.

The effects of operating conditions and parameters were investigated for selected cases. When the pre-reformed fuel is supplied, the quick drop of fuel temperature near the inlet does not occur, and hence the maximum temperature inside the cell becomes higher than in the standard case as shown in Fig. 7.

Using interconnectors with a higher thermal conductivity decreases the temperature difference inside the cell. Figure 8 displays the temperature profile for the cell with a highly thermally conducting interconnector. One can see that the temperature gradient inside the cell is apparently moderated as compared with the standard case. This effect increases the average current density, and hence the fuel utilization to 82%.

Next we focus on the effects of the gas flow pattern. When the air inlet temperature in the co-flow pattern is the same as in the standard case (counter-flow pattern), the drop of the electrolyte temperature due to the endothermic steam reforming is larger, resulting in an increase of resistance. Accordingly, the fuel utilization becomes smaller than in the standard case. In order to increase the fuel utilization to that in the standard case, the air inlet temperature has been modified to be 1173 K. All other operating conditions are the same as in the standard case. Figure 9 exhibits the temperature profile at the electrolyte in the co-flow case. In contrast to the standard counter-flow case, the electrolyte temperature increases monotonically from the fuel inlet to the fuel outlet. Although the current density profile shows a maximum value in the middle area as well as in the standard case, the difference between the maximum and the minimum current densities, 0.46 A/cm$^2$, is smaller than 0.88 A/cm$^2$ in the standard case as can be seen in Fig. 10.

Stress Calculation

Next we simulated the thermally induced stresses in the electrolyte and the interconnector. For the above-mentioned cases, the distributions of the principal stresses in the electrolyte and the interconnector were calculated from the temperature distributions. The results for the standard case are shown in Fig. 11. For all the cases, the maximum principal stresses in the interconnector are several MPa, which are low enough to avoid damage in the interconnectors. On the other hand, the principal stresses in the electrolyte are several tens MPa, and especially for the co-flow case, they reach nearly 80 MPa. When 8YSZ is used as the electrolyte, the internal stress would cause cracks or destruction of the electrolytes, since the mechanical strength
of 8YSZ sheet is not so high as 3YSZ. The tensile stress occurs near the temperature minimum point, and thus the magnitude of the maximum tensile stress can be related to the steep temperature drop caused by the prevailing steam reaction. For the external steam reforming case, the maximum tensile stress becomes one order of magnitude smaller than those for the internal steam reforming cases because there are no steep temperature drops coming from the largely endothermic reaction. Focusing on the difference between the co-flow and the counter-flow systems employing the internal steam reforming, one can find that the maximum tensile stress is smaller in the co-flow case than in the counter-flow cases. This comes from the fact that the steam reforming reaction is less prevailing than in the co-flow case, and the electrolyte temperature gradually increases along the fuel flow. It can be concluded that in terms of the tensile stress the co-flow system is more favorable than the counter-flow system. All the simulated results are summarized in Table 2.

CONCLUSIONS

The fluid flow phenomena, including heat transfer, mass transfer, and chemical reactions in the planar SOFC were simulated for the simplified single-unit model with the bipolar channels for co-flow or counter-flow pattern. The steam-reforming reaction, the water-shift reaction, and the diffusion of gases in the porous electrode were modeled. The effects of the cell size, the operating voltage, and the thermal conductivity of the cell components on the calculated results were investigated. Using the finite element method, the stress distributions in the electrolytes and the interconnectors were calculated from the simulated temperature profiles. It was found that the internal reforming would induce a steep drop of fuel temperature near the inlet, resulting in large tensile stresses in the electrolytes. The co-flow pattern is advantageous to mitigate the steep temperature gradient, and hence to reduce the internal stresses.

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**Nomenclature** (List of symbols)

\[ h = h_i + \sum m_m H_m \]
\[ t : \text{time} \]
\[ x_i : \text{Cartesian coordinate (} i = 1,2,3 \text{)} \]
\[ u_i : \text{absolute fluid velocity component in direction } x_i \]
\[ \tilde{u}_i : \text{relative velocity between fluid and local coordinate frame that moves with velocity } u_{ij} \]
\[ p : \text{piezometric pressure} \]
\[ \rho : \text{density} \]
\[ \tau_{ij} : \text{stress tensor component} \]
\[ s_i : \text{momentum source components} \]
\[ \sqrt{g} : \text{determinant of metric tensor} \]
\[ m_m : \text{mass fraction of mixture constituent } m \]
\[ H_m : \text{heat of formation of constituent } m \]
\[ h_i : \text{thermal enthalpy} \]
\[ s_i : \text{energy source} \]
\[ F_{h,j} : \text{diffusional energy flux in direction } x_j \]
\[ M_A : \text{total mass of air in the channel} \]
\[ M_F : \text{total mass of fuel in the channel} \]
\[ S_i : \text{rate of production or consumption of species } i \]
\[ H_A : \text{total enthalpy of air in the channel} \]
\[ H_F : \text{total enthalpy of fuel in the channel} \]
\[ H_S : \text{enthalpy in the electrolyte} \]
\[ Q : \text{heat source term} \]
\[ q : \text{heat loss term} \]
\[ T : \text{temperature} \]
\[ \lambda : \text{thermal conductivity} \]
\[ \kappa : \text{heat transfer coefficient} \]
\[ n : \text{unit vector normal to the boundary} \]
Table 1. The operating conditions and parameters used for the simulation.

| Sample | Velocity (m/s) | Temperature (K) | Composition | Fuel Air Channel length (mm) | Thermal conductivity (Wm⁻¹K⁻¹) | Flow pattern | Operating voltage (V) |
|--------|----------------|-----------------|-------------|-------------------------------|---------------------------------|--------------|-----------------------|
| #1     | 0.4            | 1273            | H₂O/CH₄=2   | 3                            | 1123                            | 100          | 1.8                   | 2.25                |
| #2     | 0.57           | 1273            | pre-reformed| 3                            | 1123                            | 100          | 1.8                   | 2.25                |
| #3     | 0.4            | 1273            | H₂O/CH₄=2   | 3                            | 1123                            | 100          | 10                    | 2.25                |
| #4     | 0.4            | 1273            | H₂O/CH₄=2   | 3                            | 1173                            | 100          | 1.8                   | 2.25                |
| #5     | 1.2            | 1273            | H₂O/CH₄=2   | 9                            | 1123                            | 300          | 1.8                   | 2.25                |
| #6     | 0.4            | 1273            | H₂O/CH₄=2   | 3                            | 1123                            | 100          | 1.8                   | 2.25                |

Table 2. Comparison of the simulated results.

| Sample | Fuel utilization (%) | Average current density (A/cm²) | Cell temperature (K) | Maximum tensile stress (MPa) |
|--------|----------------------|---------------------------------|-----------------------|-----------------------------|
|        |                      |                                 | at fuel outlet        | at air outlet                | maximum in separator in electrolyte |
| #1     | 79                   | 0.398                           | 1213                  | 1526                        | 1488                                      | 1.96          | 67                   |
| #2     | 77                   | 0.308                           | 1200                  | 1511                        | 1536                                      | 0.57          | 7.7                  |
| #3     | 82                   | 0.41                            | 1291                  | 1320                        | 1398                                      | 0.45          | 79                   |
| #4     | 77                   | 0.386                           | 1344                  | 1338                        | 1352                                      | 0.79          | 26                   |
| #5     | 77                   | 0.386                           | 1162                  | 1331                        | 1571                                      | 2.64          | 95                   |
| #6     | 92                   | 0.463                           | 1232                  | 1443                        | 1617                                      | 2.41          | 77                   |

Figure 1. The illustrations of the one-cell stack and the single-unit model used for the simulation.

Figure 2. The discrete anode/electrolyte/cathode unit and the equivalent circuit.
Figure 3. The calculated profiles of CH₄, H₂, CO concentrations in the anode for the standard case (#1).

Figure 4. The temperature profile in the single-unit and the electrolyte for the standard case (#1).

Figure 5. OCV profile in the anode for the standard case (#1).

Figure 6. The current density profile in the anode for the standard case (#1).

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Figure 7. The temperature profile in the electrolyte for the external-reforming case (#2).

Figure 8. The temperature profile in the single-unit for the case of using an interconnector with a higher thermal conductivity (#3).

Figure 9. The temperature profile in the electrolyte for the co-flow case (#4).

Figure 10. The current density profile in the anode for the co-flow case (#4).

Figure 11. The tensile stress profiles in the electrolyte (a) and the interconnector (b) for the standard case (#1).

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