Transient analysis of a solid oxide fuel cell stack with crossflow configuration

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Abstract. This study investigates the transient response of the cell temperature and current density of a solid oxide fuel cell having 6 stacks with crossflow configuration. A commercial software repeatedly solves the governing equations of each stack, and get the convergent results of the whole SOFC stack. The preliminary results indicate that the average current density of each stack is similar to others, so the power output between different stacks are uniform. Moreover, the average cell temperature among stacks is different, and the central stacks have higher temperature due to its harder heat dissipation. For the operating control, the cell temperature difference among stacks is worth to concern because the temperature difference will be over 10°C in the analysis case. The increasing of the inlet flow rate of the fuel and air will short the transient state, increase the average current density, and drop the cell temperature difference among the stacks. Therefore, the inlet flow rate is an important factor for transient performance of a SOFC stack.

1. Introduction

The assembly of a solid oxide fuel cell (SOFC) includes an anode, a cathode, an electrolyte and an interconnector, as well as its operating temperature is between 600 and 1000°C. Because of the high operating temperature, the SOFC can apply the methane or ethanol as its fuel. The most shapes of a SOFC unit have two, cylindrical and flat shape, and the SOFC stack with flat shape is widely in application because this shape unit is easy for stacking. Due to the high operating temperature, a SOFC always combine other faculties to promote its power output, and the transient results of a SOFC stack become more important for the system control. This study surveys the transient research on the SOFC in the recent decade [1]-[10], and finds that all literature focusing on the transient analysis of a SOFC unit with parallel configuration because of its one-dimensional mathematical model. Most of these literature investigate the effect of parameters on the transient performance [1], [2]-[3], [7], [9], others develop the model for rapid calculating the transient results in the control viewpoint. The benefit of crossflow configuration is its easier inlet arrangement, and this configuration is generally applied in the SOFC stack. However, there is few literatures focusing on its transient analysis, especially for a SOFC stack. Therefore, the results of this study can provide a valuable information for the control of a SOFC operation.

2. Analysis

The schematic of a SOFC stack with crossflow configuration is shown in Fig. 1. This study considers that the gas in each channel is laminar and slug flow. Due to the repeating layers of SOFC stack, this study builds the governing equations for each layer, and then repeatedly calculates these stacking layers. In each layer, authors consider the anode, cathode, and electrolyte as a one component named the cell. Moreover, the variety in z direction is neglected because the length scale in thickness is smaller than that in the x and y direction, so this analysis is two-dimensional problem.
The governing equations of each layer include the reaction equations, mass conservation equations, energy conservation equations, electrochemical equations.

### 2.1 Reaction equations

1. \[ \text{H}_2 + \text{O}^{2-} \rightarrow \text{H}_2\text{O} + 2\text{e}^- \]
2. \[ \text{O}_2 + 4\text{e}^- \rightarrow 2\text{O}^{2-} \]

### 2.2 Mass conservation equations

In the fuel side,

\[
\frac{d}{dt} \left( \frac{P \cdot R \cdot T_f \cdot X^k_j}{x_j} \right) + \frac{d}{dx} \left( \frac{n_f^k \cdot X^k_j}{l_y} \right) = S^k_j
\]

In the air side,

\[
\frac{d}{dt} \left( \frac{P \cdot R \cdot T_a \cdot X^k_j}{x_j} \right) + \frac{d}{dy} \left( \frac{n_a^k \cdot X^k_j}{l_x} \right) = S^k_j
\]

Meanwhile, \( n_f = N_f / l_y \) and \( n_a = N_a / l_x \). The fuel and air are ideal gas, and \( S_j \) stands for the reaction rate of reactants and products in the following:

\[
S_{\text{H}_2} = -i/(2F), S_{\text{H}_2\text{O}} = i/(2F), S_{\text{O}_2} = -i/(4F)
\]

### 2.3 Energy conservation equations

In the fuel side,

\[
\frac{d}{dt} \left( \frac{P \cdot X^k_j \cdot c_p \cdot T_c^k}{x_j} \right) + \frac{d}{dx} \left( \sum \left( n_f^k \cdot X^k_j \cdot c_p \cdot T_f^k \right) / l_x \right) = (ha)_f(T_f^k - T_c^k) + (ha)_c(T_f^k - T_c^k) + i/(4F) \cdot c_{p,03}^2 \cdot T_c^k
\]

In the air side,

\[
\frac{d}{dt} \left( \frac{P \cdot X^k_j \cdot c_p \cdot T_a^k}{x_j} \right) + \frac{d}{dy} \left( \sum \left( n_a^k \cdot X^k_j \cdot c_p \cdot T_a^k \right) / l_x \right) = (ha)_a(T_a^k - T_c^k) + (ha)_c(T_a^k - T_c^k) - i/(4F) \cdot c_{p,03}^2 \cdot T_a^k
\]

In the cell,

\[
d(\rho_c \cdot \delta_c \cdot c_{p,0} \cdot T_c^k) / dt - (k \delta)_c(\partial^2 T_c^k / \partial x^2 + \partial^2 T_c^k / \partial y^2) =
\]
\begin{equation}
(k)_{ic}(T_{ic}^{k} - T_{ic}^{c})/\delta_{ic} + (k)_{ic}(T_{ic}^{k-1} - T_{ic}^{c})/\delta_{ic} + (ha)_{cf}(T_{ic}^{k} - T_{ic}^{c}) + (ha)_{ca}(T_{ic}^{k} - T_{ic}^{c}) + i/(4F) \cdot c_{p,\text{air}}T_{ic}^{k} - i/(4F) \cdot c_{p,\text{air}}T_{ic}^{c} + q_{\text{reaction}}
\end{equation}

In the interconnector
\begin{equation}
d(\rho_{i}(\delta_{i}c_{p,\text{air}}T_{ic}^{k})/dt - (k)_{i}(\delta_{i}^{2}T_{ic}^{k}/\delta x^{2} + \delta_{i}^{2}T_{ic}^{k}/\delta y^{2}) = (k)_{ic}(T_{ic}^{k} - T_{ic}^{c})/\delta_{ic} + (k)_{ic}(T_{ic}^{k+1} - T_{ic}^{k})/\delta_{ic} + (ha)_{i}(T_{ic}^{k+1} - T_{ic}^{k}) + (ha)_{a}(T_{ic}^{k+1} - T_{ic}^{k})
\end{equation}

The subscript f is the fuel, a is the air, i is the interconnector, c is the cell, and the superscript k stands for the layer number. The initial, inlet, and boundary conditions are in the following:
\begin{equation}
\partial^{2}T_{ic}^{k}/\partial x^{2} = \partial^{2}T_{ic}^{k}/\partial y^{2} = 0, \quad \partial^{2}T_{ic}^{h}/\partial x^{2} = \partial^{2}T_{ic}^{h}/\partial y^{2} = 0
\end{equation}
\begin{equation}
T_{\text{initial}} = T_{\text{top}}^{\text{inlet}} = T_{\text{bottom}}^{\text{inlet}} = T_{\text{inlet}} = T_{\text{a,inlet}} = T_{0}
\end{equation}

2.4 Nernst equation and polarization equations
\begin{equation}
E^{k} = V^{k} + V_{\text{ohm}}^{k} + V_{\text{act}}^{k} + V_{\text{con}}^{k}
\end{equation}
\begin{equation}
E^{k} = E_{0}^{k} + (R T_{c}^{k})/(2F) \ln \left(p_{H_{2}O}^{k}/p_{H_{2}O}^{0.5}\right)
\end{equation}
\begin{equation}
E_{0}^{k} = 1.2723 - 2.7654 \times 10^{-4} T_{c}^{k}
\end{equation}
\begin{equation}
V_{\text{ohm}}^{k} = i r_{s}^{k}
\end{equation}
\begin{equation}
V_{\text{act}}^{k} = (R T_{c}^{k})/(2F) \sinh^{-1} \left(i^{k}/(2I_{0,\text{anode}}^{k})\right) + (R T_{c}^{k})/(2F) \sinh^{-1} \left(i^{k}/(2I_{0,cathode}^{k})\right)
\end{equation}
\begin{equation}
V_{\text{con}}^{k} = -(R T_{c}^{k})/(2F)
\end{equation}
\begin{equation}
\ln \left(1 - (R T_{c}^{k})/(2F) \cdot \left(\delta_{\text{anode}}/D_{\text{anode}}H_{2}^{k} \cdot i^{k}\right) / \left(1 + (R T_{c}^{k})/(2F) \cdot \left(\delta_{\text{anode}}/D_{\text{anode}}H_{2}^{k} \cdot i^{k}\right)\right)\right)
\end{equation}

Meanwhile, $r_{s} = 300 \times 10^{-7} \text{ } \Omega \text{ } \text{m}^{2}$, $I_{0,\text{anode}} = 1290 \text{ } \text{Am}^{-2}$, $I_{0,\text{cathode}} = 970 \text{ } \text{Am}^{-2}$, $\delta_{\text{anode}} = 0.05 \text{ } \text{mm}$, $D_{\text{anode}} = 2 \times 10^{-6} \text{ } \text{ms}^{-1}$ [11].

3. Simulation
Authors have published some papers investigating the steady performance of the SOFC unit and stack by using both Fortran code developed by authors and the FlexPDE software [12]-[14], and have proved the reliability of this commercial software FlexPDE. Therefore, this study applies the software to solve the Eqns. (1) to (17) to get the unknown variables depending on the time and position, such as the molar fraction of the fuel and air, the temperature of fuel, air, cell, and interconnector, as well as the current density. For accuracy comparison, this study selects the same parameters of the analysis case in previous literature [13], [14] to run the steady and transient program for a SOFC unit. In the transient analysis program, the calculating time is from 0 to 1000s. Figure 2 and 3 show the current density and cell temperature distribution in the 200, 600s, and the steady state. In these figures, the color distribution represents the steady state by using the steady program, and the blue line distribution represents the transient result by using the transient program. The two figures indicate that the results of transient program match well with the results of steady program after 600s.

![Figure 2. Comparison of current density of a SOFC unit in transient and steady](image-url)
4. Results and Discussion
This study analyzes a SOFC stack with 6 layers, and the fuel composition is H$_2$(50%) and CO$_2$(50%) as well as the air composition is O$_2$(21%) and N$_2$(79%). The inlet temperature of fuel and air is 900°C, and the molar flow rate of fuel and air inlet is 0.00023 and 0.01177 mol/s [15]. The operation voltage in this analysis case is 0.7V. Figure 4 shows the average current density of each layer from 0 to 600s. In this figure, it is obvious that the average current densities of every layer are similar, so the power output of each layer is uniform. Moreover, the SOFC stack gets the steady state at 600s in this analysis case.

Figure 3. Comparison of cell temperature of a SOFC unit in transient and steady

Figure 4. Response of average current density of each layer

Figure 5 shows the average cell temperature and cell temperature at the center of each layer from 0 to 600s. In Fig. 5(a), the layer 3 and 4 (blue lines) have the highest temperature, and the layer 1 and 6 (red lines) have the lowest temperature comparing to other layers. Because the reaction heat in the central layers is hard to spread out, the central layers must have higher temperature. In Fig. 5 (b), the temperature at cell center is slightly higher than that of average cell temperature of each layer, but the time getting steady state of temperature at cell center is shorter than that of average cell temperature. In Figs. 5(a) and 5(b), the temperature difference at different layers can be 12°C at near 100s, and be 8°C at steady state. Therefore, the cell temperature distribution in different layer of a SOFC stack in transient and steady state is worth to concerned.
Figure 5. Response of cell temperature of each layer

Figure 6 shows the average current density of the 3rd layer at one, two, and three times of original inlet molar flow rate of the fuel and air. In this figure, it is obvious that the increasing inlet molar flow rate will short the transient state, and increases the average current density. The time getting the steady state drops from 400s to less than 100s when the inlet flow rate is four times. Therefore, the change of inlet flow rate strongly affects the time getting the steady state, and it is an important factor in control viewpoint.

Figure 7 depicts the average cell temperature of the 1st, 2nd, and 3rd layer in the SOFC stack at different inlet molar flow rates. Meanwhile, the continuous, dashed, and dash-dotted line represent the one, two, and four times of the original inlet flow rate of the fuel and air, respectively. The red, green, and blue line represents the 1st, 2nd, and 3rd layer of the SOFC stack. The results show that the increase of inlet molar flow rate not only shorts the transient state, but also drops the temperature difference among the layers. The increase of fuel and air can provide more reactants for the electrochemical reaction, as well as carry away more reaction heat from the cells. Although it seems that the increasing of fuel and air can promote the average current density in Fig. 6, and drops the cell temperature difference among the layers in Fig. 7; the fuel increasing is not a reasonable decision because of considering the fuel economy. However, the air increasing is a suitable method for decreasing the cell temperature difference in the SOFC stack.
to solve the mass equations, energy equations, and electrochemical equations of a SOFC with 6 stacks, as well as calculates the transient difference among the layers. Consequently, the inlet flow rate is an important factor getting steady state.

Conclusions
This study applies a reliable commercial software, FlexPDE, to solve the mass equations, energy equations, and electrochemical equations of a SOFC with 6 stacks, as well as calculates the transient difference among different layers. Therefore, the cell temperature variation in stacks is worth concern. Moreover, the increasing of inlet flow rate will short the time to getting steady state, increase the average current density of each layer, and drop the cell temperature difference among the layers. Consequently, the inlet flow rate is an important factor affecting the transient performance of a SOFC stack.

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