

Effects of water-gas shift reaction on simulated performance of a molten carbonate fuel cell

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Abstract

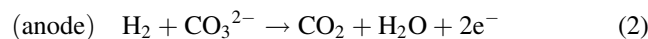
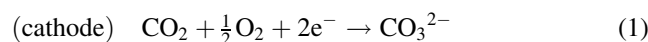
A molten carbonate fuel cell (MCFC) is simulated. In order to determine the effects of the water-gas shift reaction, the calculated results such as temperature distribution, voltage distribution, conversion and performance, are compared with those calculated excluding the shift reaction. Uniformity in the temperature profile is deteriorated due to the shift reaction. At the entrance, hydrogen is consumed rapidly in order to reach the equilibrium state of the shift reaction. The conversion of hydrogen decreases along the direction of gas flow because of hydrogen generated by the shift reaction. Therefore, when the shift reaction is excluded, the conversion of hydrogen is higher than that in a practical cell. Additionally, at the same current density, the voltage calculated without the shift reaction would be higher than the real value. The effect of the shift reaction on the voltage distribution and cell performances is quite small. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Molten carbonate fuel cell; Water-gas shift reaction; Temperature distribution; Hydrogen conversion; Cell performances

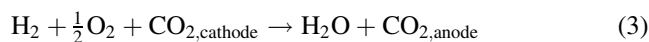
1. Introduction

The molten carbonate fuel cell (MCFC) is generally considered as a second-generation fuel cell. Coal gas, methane or carbon monoxide can be used for fuel. The MCFC operates at a high-temperature, i.e. about 650°C, so that it is able to accelerate the electrochemical reaction without a Pt catalyst. The working voltage of the MCFC is higher than that of the phosphoric acid fuel cell (PAFC), and the efficiency of generating electricity is superior because waste heat can be recovered by recycling the gases.

Reactions involved in the MCFC are the reduction of oxidant gas and the oxidation of fuel gas. The oxidant gas, containing oxygen and carbon dioxide, is supplied to the cathode and forms carbonate ions, as in Eq. (1). These ions are transported to the anode where they are involved in the oxidation of hydrogen through the molten carbonate electrolyte, as in Eq. (2). In the anode reaction, water and carbon dioxide are formed:



From Eqs. (1) and (2), the overall reaction is



A significant advantage of a high-temperature fuel cell such as MCFC is its ability to utilize CO as a fuel. When hydrogen and CO are included in the anode gas, the anodic oxidation of CO is slow compared to the anodic oxidation of H₂. Thus, the direct oxidation of CO is not likely. The following water-gas shift reaction, however, rapidly reaches an equilibrium at 650°C to produce H₂:



As H₂ is consumed in the anodic reaction (Eq. (2)), the water-gas shift reaction is driven to the right to reach an equilibrium since both H₂O and CO₂ are produced in equal quantities. Because of the shift reaction, the utilization of fuel in MCFC can exceed the utilization of H₂, based on the inlet concentration of H₂. The improved utilization of fuel is possible because the shift reaction provides the additional fuel, i.e. H₂, in the anode gas [1].

Since the water-gas shift reaction is rapid in the presence of a metal such as nickel, the following equilibrium relationship for this reaction is easily attained [2]:

$$K_S = \frac{(p_{\text{H}_2})(p_{\text{CO}_2})}{(p_{\text{H}_2\text{O}})(p_{\text{CO}})} \quad (\approx 2 \text{ at } 650^\circ\text{C}) \quad (5)$$

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| Nomenclature | |
|----------------------|---|
| b | cell thickness (cm) |
| C_p | heat capacity (J/g mol K) |
| F | Faraday's constant (96501 C/eq., 26.8 Ah/mol) |
| G | moles of gas generated and consumed per unit width (g mol/cm) |
| h | heat transfer coefficient (J/cm ² h K) |
| H | molar enthalpy (J/mol) |
| i | current density of the cell (mA/cm ²) |
| k | thermal conductivity (J/cm h K) |
| m | molar flow rate (g mol/cm h) |
| n | molar rate (g mol/h) |
| P | pressure (atm) |
| q | heat of generation per unit cell area (J/cm ²) |
| Q | heat of generation per hour (J/h) |
| R | gas constant (82.06 cm ³ atm/g mol K, 8.314 J/g mol K) |
| R_{Ohm} | Ohmic cell resistance (Ω) |
| T | temperature (K) |
| V | cell operating potential (V) |
| V_N | equilibrium potential in Eq. (8) (V) |
| V^0 | standard potential (V) |
| W | width of the fuel cell (cm) |
| x | distance in the direction of anode gas flow (cm) |
| X_k | mole fraction of the gas component k |
| y | distance in the direction of cathode gas flow (cm) |
| z | effective cell resistance (Ω cm ²) |
| <i>Greek symbols</i> | |
| η_a | anodic over-potential (<0) (V) |
| η_c | cathodic over-potential (>0) (V) |
| ν | the reaction |
| <i>Subscripts</i> | |
| a | anode |
| c | cathode |
| e | electrode-electrolyte |
| E | electrochemical reaction |
| ega | between the electrode-electrolyte plate and anode gas |
| egc | between the electrode-electrolyte plate and cathode gas |
| g | gas |
| H | hydrogen |
| i | value at the inlet of the gas |
| O | oxygen |
| res | radiation between the electrode-electrolyte plate and the upper separator |
| resc | radiation between the electrode-electrolyte plate and the lower separator |
| s | separator |
| sb | between the separator and surrounding |

| | |
|--------------------|---|
| sga | between the separator and the anode gas |
| S | water-gas shift reaction |
| W | water |
| <i>Superscript</i> | |
| 0 | value at the entrance |

Up to now, in the previous mathematical modeling of the MCFC, the water-gas shift reaction was not considered when using reformed natural gas, that is, a high Btu gas [3–5]. When the cells are large, or stacked, the effects of the water-gas shift reaction become important, as explained above. This study, therefore, examines the effects of the water-gas shift reaction on the performance of a 100 cm² unit fuel cell which uses high Btu gas as fuel. Through mathematical modeling, the temperature and current density distributions, the conversion of gases, and the performance of the fuel cell are evaluated, and the data are compared with those calculated without the shift reaction.

2. Mathematical modeling

2.1. Assumptions

In this modeling, gases flow in a way such that the anode gas (fuel gas) flows in the x -direction and the cathode gas (oxidant gas) in the y -direction. Channels are ignored and the cross-sections of the gas flows are assumed to be rectangular. Gradients of temperature along the thicknesses of the separator, gas flow channels and the electrode-electrolyte plate are neglected, since their thicknesses are smaller than their lengths and widths. Concentrations of gases in the direction of thickness are also assumed to be uniform. The cell is assumed to operate at a steady-state and the walls of the cell are assumed to be adiabatic. The absorption of the radiation energy, exchanged between the separator and the electrode-electrolyte plate, by the anode and the cathode gases is ignored [4,5].

2.2. Equations of mass balance

The equation of the mass balance of the anode gas, including the water-gas shift reaction, is as follows:

$$\frac{1}{W} \frac{\partial(n_a X_k)}{\partial x} + \nu_{E,k} \frac{i}{2F} + \nu_{S,k} \frac{n_S}{\Delta x \Delta y} = 0 \quad (6)$$

where W is the width of the cell, F the Faraday constant, viz. 26.8 Ah/mol, $\nu_{E,k}$ and $\nu_{S,k}$ are the stoichiometric coefficients of the k th component in the electrochemical reaction and the water-gas shift reaction, respectively, X_k the mole fraction of k th component, n_S (mol/h) the molar rate of generation or consumption of hydrogen by the water-gas shift reaction in the volume of ($\Delta x \Delta y b_g$), and n_a (mol/h) denotes the total anode gas flow rate which includes hydrogen and carbon monoxide. For the calculation of n_a , the hydrogen flow rate,

n_{H_2} , is calculated first using the utilization of hydrogen, u_{H} , and the total current density, i , in the following equation:

$$n_{\text{H}_2} = \frac{i/2F}{u_{\text{H}}} \quad (7)$$

Then, the flow rate of carbon dioxide is estimated with the ratio of hydrogen to carbon dioxide at the inlet of anode gas and n_a is the summation of n_{H_2} , n_{CO_2} , n_{CO} and $n_{\text{H}_2\text{O}}$.

The relationship between current density (i) and cell voltage (V) is written as [6]

$$V = (V_{\text{cN}} - V_{\text{aN}}) - iZ \quad (8)$$

where the equilibrium potentials of anode and cathode, V_{aN} and V_{cN} , are derived from the Nernst equation [6] at 1 atm, i.e.

$$V_{\text{aN}} = V_{\text{a}}^0 + \frac{RT}{2F} \ln \left(\frac{X_{\text{aC}}X_{\text{W}}}{X_{\text{H}}} \right) \quad (9)$$

$$V_{\text{cN}} = V_{\text{c}}^0 + \frac{RT}{2F} \ln(X_{\text{cC}}X_{\text{O}}^{1/2}) \quad (10)$$

where V_{a}^0 and V_{c}^0 are standard potentials, and X the compositions of each gas. Substituting V_{cN} and V_{aN} in Eq. (8) gives

$$V = (V_{\text{a}}^0 - V_{\text{c}}^0) + \frac{RT}{2F} \ln \left(\frac{X_{\text{cC}}X_{\text{O}}^{1/2}X_{\text{H}}}{X_{\text{W}}X_{\text{aC}}} \right) - iZ \quad (11)$$

The effective cell resistance, Z , in Eq. (11), is expressed by

$$Z = R_{\text{Ohm}} + \frac{\eta_{\text{a}}}{i} - \frac{\eta_{\text{c}}}{i} \quad (12)$$

The anodic and cathodic over-potentials, η_{a} and η_{c} in Eq. (12), are obtained by multiplying the current density (i) by the polarization resistances (Z_{a} and Z_{c}), namely

$$\eta_{\text{a}} = i_{\text{a}}Z_{\text{a}} = iZ_{\text{a}} \quad (13)$$

$$\eta_{\text{c}} = i_{\text{c}}Z_{\text{c}} = -iZ_{\text{c}} \quad (14)$$

In order to quantify the polarizations at the anode and the cathode, Selman [7] reported:

$$Z_{\text{a}} = 2 \times 0.4567 \times 10^{-7} (p_{\text{H}_2})^{-1.801} (p_{\text{CO}})^{1.533} (p_{\text{CO}_2})^{-1.480} \times \exp \left(\frac{13\,140}{T} \right) \quad (15)$$

$$Z_{\text{a}} = 7.504 \times 10^{-6} (p_{\text{O}_2})^{-0.43} (p_{\text{CO}_2})^{-0.09} \exp \left(\frac{9361}{T} \right) \quad (16)$$

The Ohmic cell resistance, R_{Ohm} in Eq. (12), is evaluated as a function of temperature [8].

2.3. Equations of energy-balance

The same equations of energy which have been studied previously are used [4,5].

For the upper separator:

$$\frac{\partial^2 T_{\text{s}}}{\partial x^2} + \frac{\partial^2 T_{\text{s}}}{\partial y^2} = \frac{h_{\text{res}}}{b_{\text{s}}k_{\text{s}}} (T_{\text{s}} - T_{\text{e}}) + \frac{h_{\text{sga}}}{b_{\text{s}}k_{\text{s}}} (T_{\text{s}} - T_{\text{ga}}) + \frac{h_{\text{sb}}}{b_{\text{s}}k_{\text{s}}} (T_{\text{s}} - T_{\text{b}}) \quad (17)$$

boundary condition 1 :

$$\text{at } x = 0 \text{ and } x = L, \text{ for all } y; \quad \frac{\partial T_{\text{s}}}{\partial x} = 0$$

boundary condition 2 :

$$\text{for all } x, y = 0 \text{ and } y = W; \quad \frac{\partial T_{\text{s}}}{\partial y} = 0$$

where the left-hand terms are heat transfer in the x - and y -directions by conduction. The right-hand terms are radiation heat transfer between the separator and the electrode-electrolyte plate, convective heat transfer between the separator and the anode gas, and convective heat transfer between the separator and the surrounding of the cell, respectively. A similar equation can be written for the lower separator.

The heat of the shift reaction (Q_{S}) is included in the following energy-balance equation for the anode gas:

$$\frac{\partial}{\partial x} (m_{\text{a}} C_{\text{pa}} T_{\text{ga}}) = h_{\text{ega}} (T_{\text{e}} - T_{\text{ga}}) + h_{\text{sga}} (T_{\text{s}} - T_{\text{ga}}) + \sum_k G_{\text{ai}} C_{\text{pa},k} b_{\text{g}} T_{\text{ga}} + Q_{\text{S}} \quad (18)$$

boundary condition : at $x = 0$, for all y ; $T_{\text{ga}} = T_{\text{i}}$

where the left-hand term represents the change of energy of the gas. The first two terms on the right-hand are convective energy transfers between the electrode-electrolyte plate and anode gas, and between the separator and anode gas, respectively. The third term is the change of energy by the enthalpy of each component generated or consumed by the reaction. The last term is the heat of the shift reaction. The equation for the cathode gas can be written similarly as Eq. (18) after removing Q_{S} . The heat of reaction for the shift reaction, Q_{S} (J/h) in Eq. (18), is as follows:

$$Q_{\text{S}} = \Delta H_{\text{S}} \Delta n_{\text{CO}} \quad (19)$$

where Δn_{CO} (mol/h) is the consumption rate of CO by the shift reaction and ΔH_{S} (J/mol), the heat of shift reaction, is calculated as a function of temperature [2]:

$$\Delta H_{\text{S}} = -9932.5 - 0.515T + (3.117 \times 10^{-3})T^2 - (1.05 \times 10^{-6})T^3 \quad (20)$$

For the electrode-electrolyte plate:

$$\frac{\partial^2 T_{\text{e}}}{\partial x^2} + \frac{\partial^2 T_{\text{e}}}{\partial y^2} = \frac{h_{\text{res}}}{b_{\text{e}}k_{\text{e}}} (T_{\text{e}} - T_{\text{s}}) + \frac{h_{\text{resc}}}{b_{\text{e}}k_{\text{e}}} (T_{\text{e}} - T_{\text{s}}) + \frac{h_{\text{ega}}}{b_{\text{e}}k_{\text{e}}} (T_{\text{e}} - T_{\text{ga}}) + \frac{h_{\text{egc}}}{b_{\text{e}}k_{\text{e}}} (T_{\text{e}} - T_{\text{gc}}) + \frac{q_{\text{E}}}{b_{\text{e}}k_{\text{e}}} \quad (21)$$

boundary condition 1 : at $x=0$ and $x=L$, for all y ; $\frac{\partial T_{\text{e}}}{\partial x} = 0$

boundary condition 2 : for all $x, y=0$ and $y=W$; $\frac{\partial T_{\text{e}}}{\partial x} = 0$

The left-hand terms are conductive heat transfer in the x - and y -directions in the electrode-electrolyte plate. The

Table 1
Dimensions of molten carbonate fuel cell used in mathematical modeling

| | |
|----------------------------------|------|
| Length, L (cm) | 10 |
| Width, W (cm) | 10 |
| Thickness | |
| Separator, b_s (cm) | 0.2 |
| Gas channel, b_g (cm) | 0.2 |
| Anode electrode, b_{ea} (cm) | 0.07 |
| Electrolyte plate, b_{em} (cm) | 0.1 |
| Cathode electrode, b_{ec} (cm) | 0.06 |

Table 2
Flow rates and compositions of anode and cathode gas flowing into fuel cell

| | Flow rate (mol/h) | Compositions | |
|-------------|-------------------|------------------|------|
| Anode gas | 0.875 | H ₂ | 0.68 |
| | | CO ₂ | 0.08 |
| | | CO | 0.12 |
| | | H ₂ O | 0.12 |
| Cathode gas | 1.050 | O ₂ | 0.33 |
| | | CO ₂ | 0.67 |

two right-hand terms are radiation heat transfers between the upper separator and the electrode-electrolyte plate, and between the lower separator and the electrode-electrolyte plate, respectively. The third and fourth terms are convective heat transfers between the electrode-electrolyte plate and anode gas, and between the electrode-electrolyte plate and cathode gas, respectively. The heat of electrochemical reaction, q_E (J/cm²), is obtained as follows [9]:

$$q_E = i \left(-\frac{\Delta H_E}{2F} + V \right) \quad (22)$$

where ΔH_E (J/mol) is the enthalpy change by the electrochemical reaction [2]:

$$\Delta H_E = -57018 - 2.738T + (0.474 \times 10^{-3})T^2 + (2.637 \times 10^{-6})T^3 \quad (23)$$

2.4. Conditions for the calculation

Values of parameters and dimensions of the cell are shown in Tables 1 and 2. The area of the cell is 100 cm². The flow rate of anode gas to the cell is estimated by using the utilization of hydrogen (u_H), 0.4, and the total current density (i), 150 mA/m², as in Eq. (7). Dividing the cell area into 20 × 20 grids, we calculate equations of mass and energy-balances by the finite difference method.

3. Results and discussion

In this study, the simulation of a unit MCFC is performed. We predict temperature distribution, current density distri-

bution, conversion and performance. In order to observe the effects of the shift reaction, we compare these features with those calculated in the absence of the shift reaction.

3.1. Effect of shift reaction on temperature and voltage distributions

Fig. 1 shows temperature distribution in the upper separator in (a) the presence of the shift reaction and (b) the absence of the shift reaction at 150 mA/cm². Because the upper separator is connected to the anode gas, its temperature increases along the anode gas flow, but shows little change along the cathode gas flow. The temperature gradient at the inlet of the cell is large due to the low inlet temperature (813 K) and a high fraction of H₂ in the anode gas flow into the cell. In the cross-flow type of fuel cell, the heat generated by reactions is transferred to the outlet of the anode gas, and thus, the temperature of anode gas at the outlet is much higher. Differences in temperature distribution due to the shift reaction are not very large, since the heat generated or

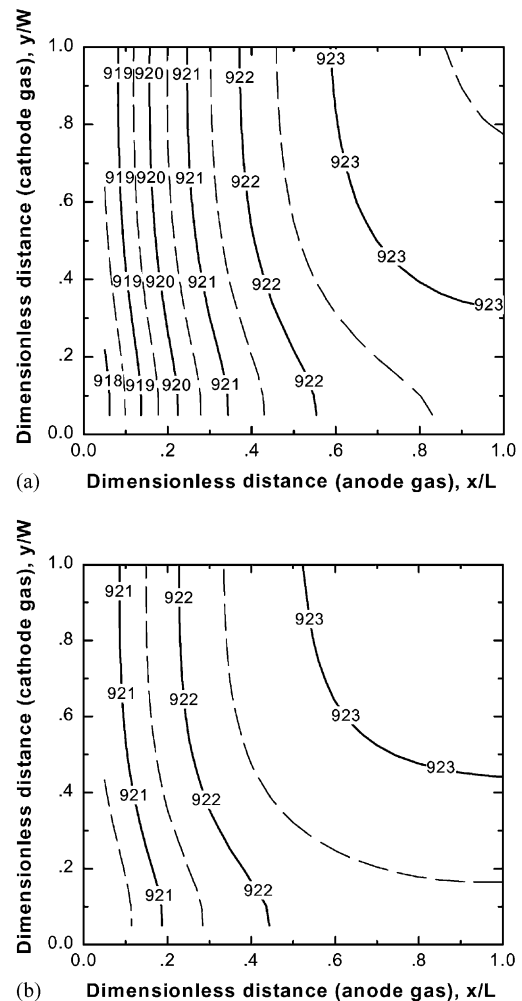


Fig. 1. Temperature contour graphs of upper separator at 150 mA/cm²: (a) including the water-gas shift reaction; (b) excluding the water-gas shift reaction.

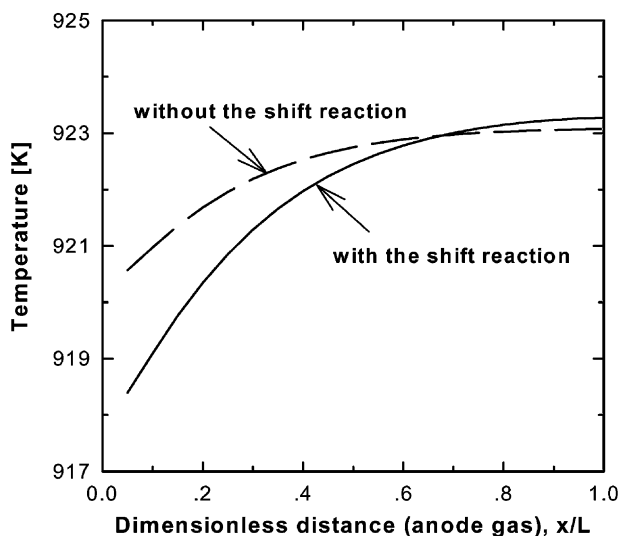


Fig. 2. Temperature distributions of upper separator along anode gas flow at center of cell ($y = 0.5 l$).

consumed by the shift reaction is smaller than that by the electrochemical reaction. The heat generated by the electrochemical reaction, ΔH_E , and the shift reaction, ΔH_S , at 923 K is $-246\,600$ and $-35\,900$ J/mol, respectively. The shift reaction, however, consumes a substantial amount of hydrogen around the inlet of the anode gas and the temperature becomes low. The effects of the shift reaction on the temperature profiles in Fig. 1 can be identified easily in Fig. 2. The temperature profiles of the upper separator along the anode gas flow at the center of the cell ($y = 0.5 l$) are shown in Fig. 2. Temperature is higher near the entrance and lower near the exit when the shift reaction is excluded. Due to the shift reaction, the temperature profile shows less uniformity.

Temperature distributions of the electrode-electrolyte plate are obtained in the same way, see Fig. 3. When the

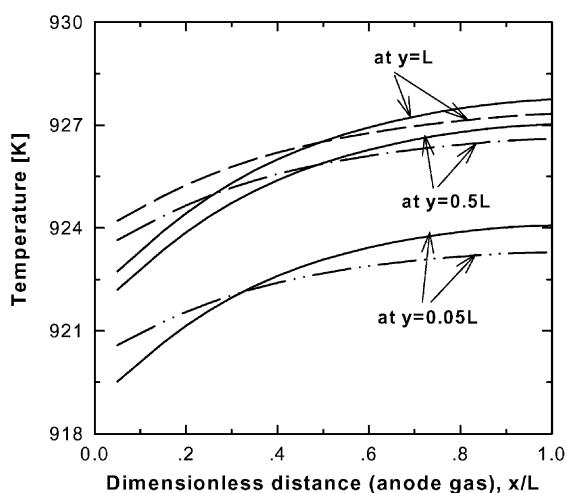


Fig. 3. Temperature distributions of electrode-electrolyte plate along anode gas flow at 150 mA/cm^2 . Solid lines are results calculated with shift reaction and dotted lines are those without shift reaction.

shift reaction is included, the amount of hydrogen decreases due to consumption near the entrance, and then increases due to generation near the exit by the shift reaction. Accordingly, heat is consumed near the entrance and generated near the exit by the shift reaction. Therefore, as explained for the upper separator, the temperature calculated in the presence of the shift reaction is lower near the entrance and then becomes higher near the exit than that calculated in the absence of the shift reaction. More heat is generated by an electrochemical reaction, and therefore, the temperature of the electrode-electrolyte plate is higher than that of anode gas. The effect of the shift reaction is small, but noticeable, because the conversion of hydrogen by this reaction is small. Again, the uniformity in the temperature profile is degraded by including the shift reaction.

At constant current density the voltage distribution is shown in Fig. 4 with the shift reaction, the cell voltage lies between 0.91 and 1.02 V. When the shift reaction is not

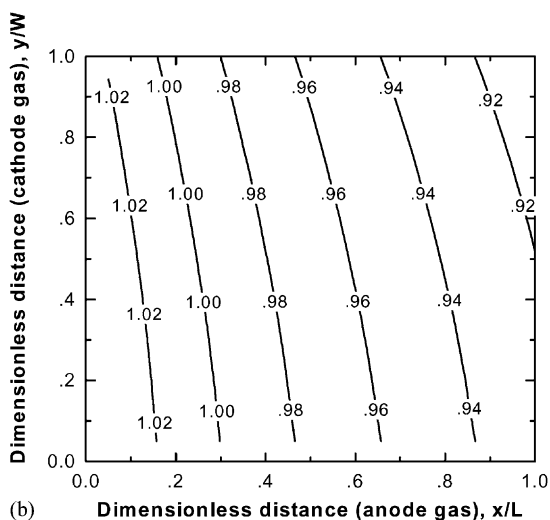
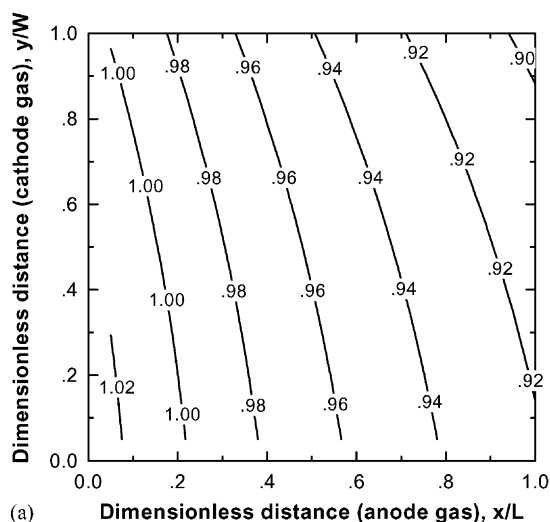


Fig. 4. Contour graphs of cell voltage distribution at constant current density, 150 mA/cm^2 : (a) with the water-gas shift reaction; (b) without water-gas shift reaction.

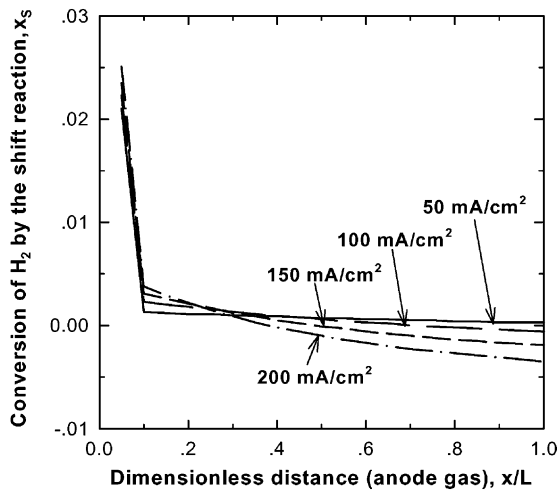


Fig. 5. Conversion of hydrogen only by water-gas shift reaction along direction of anode gas flow at different current densities.

included, the voltage is between 0.92 and 1.03 V. As the amount of hydrogen consumed by the shift reaction increases, the fraction of hydrogen decreases and voltage also decreases, as indicated by Eq. (11). Nevertheless, the voltage gradient is almost the same in both cases.

3.2. Effect of shift reaction on hydrogen conversion

The effect of the water-gas shift reaction on the conversion of anode gas are studied. The change of the local consumption of hydrogen by the shift reaction along the anode gas flow is given in Fig. 5 for current densities of 50, 100, 150 and 200 mA/cm². Here, the local consumption, x_S , is the ratio of hydrogen generated or consumed by the shift reaction to the total amount of anode gas at an arbitrary point in the cell. It has a negative value when hydrogen is generated.

The data in Fig. 5 show that the local consumption changes from a positive value to a negative one. This can be explained as follows. The shift reaction in Eq. (4) progresses reversely to reach an equilibrium state near the entrance. After reaching equilibrium, however, the reaction progresses forward so that hydrogen is generated near the exit.

The sharp slope at the inlet of the cell indicates rapid consumption of hydrogen. This is because of a rise in temperature near the entrance. If the temperature rises, the equilibrium constant of Eq. (4) decreases from 5 (at 500°C) and 2 (at 650°C) [10]. As a result, there is a sharp increase in the hydrogen consumption by the shift reaction.

Increasing the current density means consuming more hydrogen by the electrochemical reaction when the inflow of anode gas is constant. Thus, as the current density increases, the amount of carbon monoxide, shifted to hydrogen by the reaction in Eq. (4), also increases. In another words, the generation of hydrogen by the shift reaction increases. At 50 mA/cm², however, the hydrogen consumed by the elec-

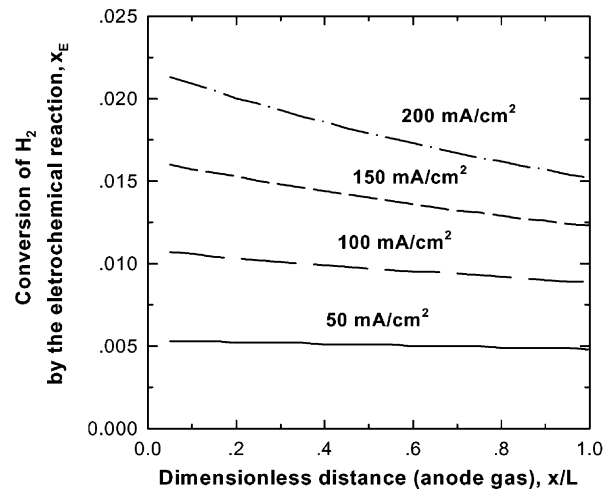


Fig. 6. Conversion of hydrogen only by electrochemical reaction along direction of anode gas flow.

trochemical reaction is so small that hydrogen is consumed by the shift reaction through the whole cell.

Similarly, Fig. 6 shows the conversion of hydrogen by the electrochemical reaction, x_E , at different current densities. Since the cell is operating at each constant current density, the amount of hydrogen consumed by the electrochemical reaction should be constant at any point in the cell. When 1 mol of hydrogen is reacted, 1 mol of water and 1 mol of carbon dioxide are produced. Thus, the total anode gas flow rate increases and the local conversion of hydrogen based on the local amount of anode gas decreases along the direction of the anode gas flow.

Changes in the total conversion of hydrogen along the anode gas flow are given in Fig. 7 and are based on the initial amount of hydrogen at the entrance, at a constant current density of 50, 100 and 150 mA/cm² including and excluding

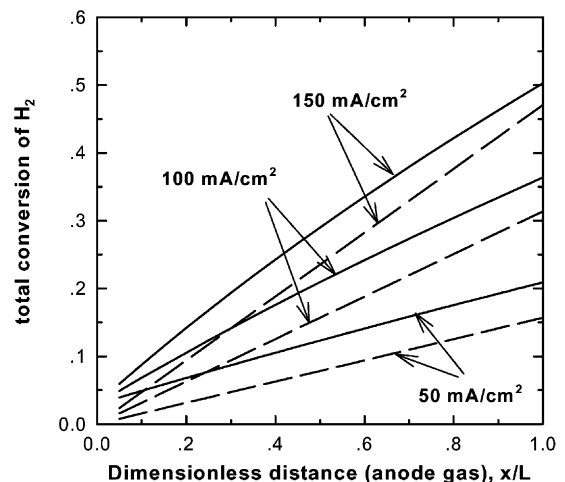


Fig. 7. Total conversion of H₂ in anode gas along direction of anode gas flow at different current densities. Solid lines are results calculated including shift reaction and dotted lines are those calculated excluding shift reaction.

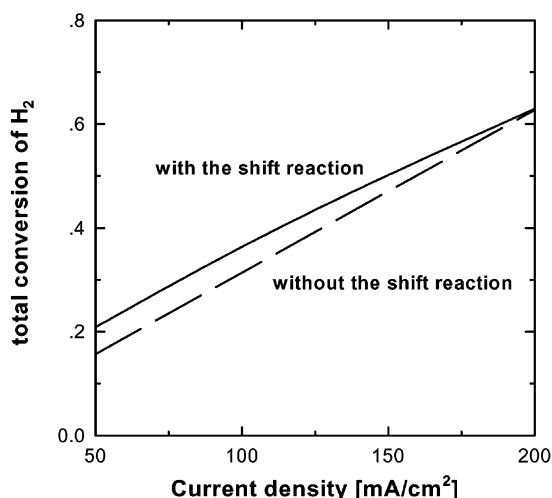


Fig. 8. Changes of total conversion of H₂ in anode gas with current density calculated with and without water-gas shift reaction.

the shift reaction. Here, the conversion of hydrogen is defined as the fraction of hydrogen consumed or generated by both the electrochemical reaction and the shift reaction based on the initial amount of hydrogen.

If the shift reaction is excluded, the conversion would change almost linearly. When the shift reaction is included, however, the slope of the conversion line decreases slightly towards the exit. This is because the shift reaction in Eq. (4) progresses forward and hydrogen is generated. As we can see from Fig. 5, if the current density becomes high, the conversion of hydrogen becomes high too when the initial anode gas flow rate is constant. As a result, at a high current density, the difference between results calculated including the shift reaction and those calculated excluding the shift reaction is small.

The conversion of anode gas is compared with the current density in Fig. 8. When the shift reaction is included, the conversion of anode gas, i.e. hydrogen is high because most of hydrogen is consumed at the inlet of the cell to reach an equilibrium state through the reaction in Eq. (4), so the total conversion is high. As the current density increases, however, the differences between the two cases become small. This is because the amount of hydrogen generated by the shift reaction increases more at a high current density while hydrogen is consumed by the electrochemical reaction.

3.3. Effect of the shift reaction on cell performance

The cell performance, calculated including and excluding the shift reaction, are compared in Figs. 9 and 10. As shown in Fig. 9, the cell voltage is lower when the shift reaction is included at each constant current density. Since the shift reaction in Eq. (4) progresses reversely at the inlet of the cell, more hydrogen is consumed and the fraction of carbon monoxide increases. So, the anodic polarization is relatively large in Eqs. (13) and (15) [8] and the effective cell resistance, Z , in Eq. (12) is large. Hence, the voltage in

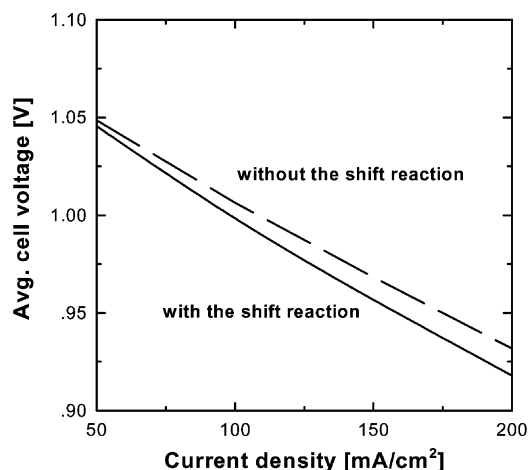


Fig. 9. Change of average cell voltage with current density calculated with and without water-gas shift reaction.

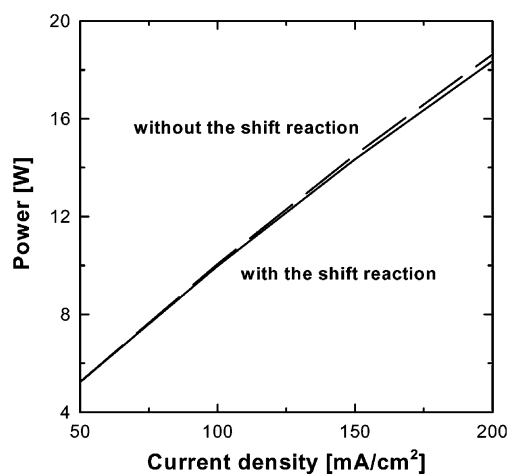


Fig. 10. Changes of power with current density calculated with and without water-gas shift reaction.

Eq. (11) becomes small. By the same reasoning, the power of the cell in Fig. 10, expressed as a multiplication of the current density and the cell voltage is low when the shift reaction is included.

4. Conclusions

Through the simulation of a unit MCFC, a study has been made of the effects of the water-gas shift reaction on temperature distribution, voltage distribution, conversion and performance. The following conclusions are obtained.

The temperature of the inlet gas is lower than that of the cell. Hence, as the temperature of the gas rises near the entrance, the shift reaction progresses reversely to reach an equilibrium state and hydrogen is consumed rapidly. Then, the shift reaction progresses forward and hydrogen is generated near the exit. This is why the temperature calculated

with the shift reaction is lower near the entrance and then becomes higher near the exit than that calculated without the shift reaction. This is noticeable even if the effect of shift reaction on the temperature distribution is small. The uniformity in the temperature profile is degraded by the shift reaction.

The rate of the total conversion of hydrogen decreases along the anode gas flow due to the shift reaction.

The effect of the shift reaction on the voltage distribution is small. As the amount of hydrogen consumed by the shift reaction increases, the fraction of hydrogen decreases as does the voltage. The cell voltage becomes higher when the shift reaction is excluded at a constant current density.

The power of the cell is slightly higher when the shift reaction is excluded. The effect of the shift reaction on the cell performances, however, is very small.

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