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Numerical study on electric characteristics of solid oxide fuel cells

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Abstract

Numerical simulations are performed in both planar and tubular geometries of a solid oxide fuel cell to study the electric characteristics. The Navier–Stokes equations are solved with an electrochemical model developed in this paper, which is a generalized, three dimensional complete polarization electrochemical model for solid oxide fuel cells with various geometries. This study conducts detailed analyses of the electric polarizations for both planar and tubular solid oxide fuel cells and presents the characteristics of the density and the potential distribution in the electric components for the planar co-flow solid oxide fuel cell. The ohmic heats in the planar and tubular configuration solid oxide fuel cell are also compared and discussed.

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Keywords: Solid oxide fuel cell; Numerical simulation; Electric characteristics

1. Introduction

A fuel cell is an energy conversion device that converts chemical energy into electrical energy through electrochemical reactions. It has become more and more promising for its high efficiency and low emission. Of all existing fuel cells, the solid oxide fuel cell (SOFC) with planar, monolithic and tubular geometries, as a high temperature fuel cell, is suitable for power generation. Most SOFC components are made of conductive materials. It is well known that the potential from the electrochemical reaction is not uniform at the electrolyte interface. Materials and geometric configurations for the SOFC also affect the fuel cell performance. It is very important to obtain the performance of current flow and potential distribution in the electric components in order to perform optimal design and obtain the operation performance of the SOFC.

Numerical studies have been conducted by different investigators on performance analysis of the SOFC, for example Refs. [1–8]. The interconnector, anode, electrolyte and cathode of the SOFC are conductive, while the electric

current in the SOFC is considered to be a flowing medium with three dimensional flows. The three dimensional characteristics of the current have a strong influence on the electric potential distribution of the SOFC. Therefore, the electric potential equation should be solved throughout the electric field in order to analysis accurately the electrical characteristics of the SOFC. The three dimensional characteristics of the electric current were not considered in most of the models used in previous studies [1-6]. Very often, the Tafel equation or linear current-voltage relation was used to replace the Butler-Volmer equation in the calculation of the activation overpotential, or the Knudsen diffusion was neglected in the gas diffusion through the porous electrodes. Those simplifications used in previous studies will introduce errors in the numerical model for most cases. For example, as in Ref. [6], the developed numerical model results showed that there was a 17% error with the experimental result at the lower current density. The complete polarization model was just used to qualitatively analyze the solid oxide fuel cell performance [9]. The accuracy of the model needs to be validated for various geometries of SOFC.

A three dimensional numerical model of SOFCs for various geometries with complete polarization is developed in

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Nomenclature

A_0	coefficient of conductivity ($\Omega^{-1} \text{ m}^{-1} \text{ K}$)	\boldsymbol{S}
a_1	fitting function coefficient of specific heat capac-	Т
	ity $(J \text{ mol}^{-1} \text{ K}^{-1})$	t
a_2	fitting function coefficient of specific heat capac-	V
	$(I \text{ mol}^{-1} \text{ K}^{-2})$	w
<i>(</i>]2	fitting function coefficient of specific heat capac-	r
uz	ity $(I \text{ mol}^{-1} K^{-3})$	7
1	specific surface area of control volume (m^{-1})	2e
$A_{\rm CV}$	specific surface area of control volume (m) (m^{-3})	Creat
С, с	concentration (mol m) $(\mathbf{L} = \mathbf{L}^{-1} \mathbf{K}^{-1})$	Gree
c_p	specific field capacity (J filot K) diffusion acofficient $(m^2 a^{-1})$	α
	$\frac{1}{1}$	р
E	activation energy (J mol)	η
E_0	coefficient of conductivity (K)	ho
$E_{\rm v}$	voltage (V)	σ
E_{n}	Nernst potential (V)	ψ
F	Faraday constant (=96485 A s mol ⁻¹)	Φ
f_{e}	equilibrium factor for reforming reaction	ϕ
g	molar Gibbs free energy (J mol ⁻¹)	Γ
ΔG	change of Gibbs free energy for chemical reac-	ζ
	tion $(J \text{ mol}^{-1})$	λ
h	molar enthalpy $(J \text{ mol}^{-1})$	γ
ΔH	change of enthalpy for chemical reaction	
	$(J \text{ mol}^{-1})$	μ
i	current density (A m^{-2})	
i_0	exchange current density (A m^{-2})	Subs
J, j	flux (mol s^{-1})	а
K	equilibrium constant	act
k	rate of reaction (mol s^{-1}), stoichiometric reac-	b
	tion coefficient	с
k_0	constant parameter for rate of reforming reac-	chen
0	tion (mol s ⁻¹ m ² p ₂ ⁻¹)	conc
k_1	constant parameter for rate of shift reaction	CV
	$(\text{mol } \text{m}^{-3} \text{s}^{-1})$	Ē
1	distance (m)	eff
ĩ	length of cell (m)	el
$\frac{L}{M}$	molecular mass $(kg \text{ mol}^{-1})$	f
101 1	unit normal vector of reaction interface	i
n n	electrons transferred per reaction	i i
n _e	pressure (P ₂)	J K
Р Р	standard pressure (Pa)	D
г ₀	standard pressure (Fa) rate of heat transfer (L c^{-1})	r. C
ч О	hat course $(W m^{-3})$	5 0 hrs
\mathcal{Q}	neat source (w m $^{-2}$)	onm
r ·	area specific resistance $(\Omega \text{ m}^{-1})$	р
r	volumetric reaction rate (mol s ⁻¹ m ⁻¹)	r
ĸ	universal gas constant (= $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$)	rad
$R_{\rm n}$	area specific resistance (Ωm^2)	ret
S	molar entropy $(J \text{ mol}^{-1} \text{ K}^{-1})$	tot

source component temperature (K) time (s) velocity (m s^{-1}) rate of work $(J s^{-1})$ molar fraction of gases species rate of electrons transfer (mol s^{-1}) ek letters permeability of porous material (m²) current transfer coefficient polarization (V) fluid density (kg m^{-3}) conductivity $(\Omega^{-1} m^{-1})$ entropy production $(J K^{-1} s^{-1})$ electric potential (V) generalized scalar of control equations diffusion coefficient of control equations inertial resistance factor (m^{-1}) heat conductivity (W m⁻¹ K⁻¹) kinetic parameters in Eqs. (5b) and (5c) $(A m^{-2})$ fluid viscosity (Pa s) scripts anode activation back cathode chemical reaction n concentration control volume electrochemical oxidizing reaction effective electrolyte forward chemical species direction of coordinate Knudsen diffusivity reforming reaction shift reaction ohmic products reactants radiant reference

this study. Methane reforming and the water-gas shift are included in the model. This model is coupled with the governing equations through the user defined function (UDF) interface, which was provided by the commercial CFD software, Fluent. Transport equations for mass, momentum, species, energy and electrical potential are solved using the software, Fluent. The electric characteristics of the conductive components for both planar and tubular

total

configured SOFCs are studied. The current flow, ohmic loss and polarization losses are analyzed using numerical results from the simulations.

2. Electrochemical model

The electrochemical processes in the SOFC are illustrated in Fig. 1. Fuel and air are allowed to flow into the cell separately. They diffuse through the porous electrode structure to the interlayer and are adsorbed. At the cathode interlayer, oxygen is reduced by the incoming electrons to produce oxygen anions that are conducted through the electrolyte to the anode interlayer where they electrochemically combine with the adsorbed hydrogen to form water and release electrons to the external circuit. In order to simplify the numerical model, we assume the interlayer is an interface with zero thickness. The electrochemical reactions for the anode and cathode are:

Anode side: $H_2 + O^{2-} \rightarrow H_2O + 2e^-$ Cathode side: $1/2O_2 + 2e \rightarrow O^2$ Overall reaction: $1/2O_2 + H_2 \rightarrow H_2O$.

For the internal reforming of the SOFC, the reforming reaction and water-gas shift reaction are added within the anode:

Steam reforming:
$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Shifting: $CO + H_2O = CO_2 + H_2$

Also, the electrochemical oxidation of carbon monoxide at the anode is formulated as

$$\rm CO + O^{2-} \rightarrow \rm CO_2 + 2e^-$$

However, this reaction velocity is 2–5 times slower than that of hydrogen. The rapid water-gas shift reaction becomes the dominant reaction [4]. Therefore, in the model, the oxidation of carbon monoxide is neglected.

As an energy conservation system, the energy conservation of the electrochemical reaction for the SOFC is written as

$$q - w + \sum_{i} (k_{i}h_{i})_{\rm r} - \sum_{i} (k_{i}h_{i})_{\rm p} = 0$$
 (1)

The entropy balance for the electrochemical reaction is given by



Fig. 1. Electrochemical processes within SOFC.

$$q/T - \sum_{i} (k_{i}s_{i})_{\rm r} - \sum_{i} (k_{i}s_{i})_{\rm p} + \psi = 0$$
⁽²⁾

Combining Eqs. (1) and (2) for $w = z_e F E_v$ we can obtain the following equation:

$$E_{\rm v} = -\frac{1}{z_{\rm e}F} \left[\sum_{i} (k_i g_i)_{\rm p} - \sum_{i} (k_i g_i)_{\rm r} \right] - \frac{T\psi}{z_{\rm e}F}$$
(3a)

where

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$$g_{i}(T, p_{i}) = h_{i}(T) - Ts_{i}(T, p_{i})$$

= $\int_{T_{0}}^{T} c_{pi}(T) dT - T \int_{T_{0}}^{T} \frac{c_{pi}(T)}{T} dT - RT \ln \frac{P_{0}}{p_{i}}$
(3b)

and

$$\frac{T\psi}{z_{\rm c}F} = \eta_{\rm act} + \eta_{\rm ohm} + \eta_{\rm conc}.$$
(3c)

 c_{pi} in Eq. (3b) can be expressed as follows:

$$c_{pi}(T) = a_1 + a_2 T + a_3 T^2 \tag{3d}$$

The coefficients a_1 , a_2 , a_3 , are constant and given in Table 1.

2.1. Activation polarization

The energy barrier, which is called activation polarization, exists between the electronic and the ionic conductors of the electrochemical reaction. The activation polarization occurs at both electrodes in all ranges of current densities. Generally, it is expressed by the Butler–Volmer equation:

$$i = i_0 \left\{ \exp\left(\beta \frac{n_e F \eta_{act}}{RT}\right) - \exp\left[-(1-\beta) \frac{n_e F \eta_{act}}{RT}\right] \right\}$$
(4)

In this paper, β is set to be 0.5. Then

$$\eta_{\rm act} = \frac{2RT}{n_{\rm e}F} \sinh^{-1}\left(\frac{i}{2i_0}\right) \tag{5a}$$

The exchange current density i_0 depends on the partial pressure of the reacting gas compositions and the temperature. The following equation applies according to Ref. [10]. At the anode side,

$$i_0 = \gamma_a \left(\frac{p_{H_2}}{p_{ref}}\right) \left(\frac{p_{H_2O}}{p_{ref}}\right) \exp\left(-\frac{E_a}{RT}\right)$$
(5b)

At the cathode side

$$\dot{v}_0 = \gamma_c \left(\frac{p_{O_2}}{p_{ref}}\right)^{0.25} \exp\left(-\frac{E_c}{RT}\right)$$
(5c)

Table 1

Specific	heat	canacity	coefficients	for	the	chemical	species
specific	neat	capacity	coefficients	101	the	chennear	species

	$a_1 (J/mol K)$	$a_2 \times 10^3 \; (J/mol \; K^2)$	$a_3 \times 10^6 (\text{J/mol K}^3)$
H ₂	29.0856	-0.8373	2.0138
O_2	25.8911	12.9874	-3.8644
H_2O	30.3794	9.6212	1.1848
CH_4	14.1555	75.5466	-18.0032
CO_2	26.0167	43.5259	-14.8422
CO	26.8742	6.9710	-0.8206

The temperature appeared in Eqs. (4) and (5a) is the reacting site temperature. The kinetic parameters in the equations can be evaluated by experiments. In this paper, these parameters are determined as follows [11]:

$$\gamma_{a} = 5.5 \times 10^{8} \text{ A/m}^{2}, \quad E_{a} = 1.0 \times 10^{5} \text{ J/mol},$$

 $\gamma_{c} = 7.0 \times 10^{8} \text{ A/m}^{2}, \quad E_{c} = 1.2 \times 10^{5} \text{ J/mol}.$

2.2. Concentration polarization

The electrochemical reactions occur at the electrolyte– electrode interface. However, the gas partial pressures, which are used to calculate the change of Gibbs free energy, are different from the reactions site gas partial pressures. So, corrections to account for the difference between the actual gas partial pressures and the ones used in calculating the Gibbs free energy at both the anode and the cathode are required. The corrections are generally called concentration polarization.

The reacting gas compositions diffusion to the reaction sites through the porous material of the electrodes is described by Knudsen diffusion. The concentration polarization is given as follows [9]:

$$\eta_{\text{conc},a} = -\frac{RT}{2F} \left[\ln \left(\frac{p_{\text{H}_2}}{p_{\text{H}_2}^e} \right) - \ln \left(\frac{p_{\text{H}_2\text{O}}}{p_{\text{H}_2\text{O}}^e} \right) \right] \\ = -\frac{RT}{2F} \ln \left[\frac{1 - (RTl_a |\vec{i} \cdot \vec{n}|) / (2FD_{a(\text{eff})} p_{\text{H}_2}^e)}{1 + (RTl_a |\vec{i} \cdot \vec{n}|) / (2FD_{a(\text{eff})} p_{\text{H}_2\text{O}}^e)} \right]$$
(6)

loss depends on the design and manufacture of the cell. The conductivity of the electric components is a function of temperature. It is modeled by the following equation:

$$\sigma = \frac{A_0}{T} \exp\left(-\frac{E_0}{T}\right) \tag{8}$$

Then, the ohmic losses are written as

$$\eta_{\rm ohm} = r |\vec{i} \cdot \vec{n}| = l_{\rm el} |\vec{i} \cdot \vec{n}| / \sigma \tag{9}$$

2.4. Steam reforming

Because of the high operating temperature of the SOFC, hydrogen can be produced in the interior of the SOFC. At the anode side, the methane and water vapor in the fuel gas are adsorbed into the nickel based anode and are combined to produce hydrogen. Additional hydrogen is produced when carbon monoxide, in the presence of water vapor, is catalytically shifted to carbon dioxide. The reaction rate for methane reforming has been proposed by Refs. [4,12].

$$\dot{r}_{\rm R} = k_0 A_{\rm CV} p_{\rm CH_4} f_{\rm e} \exp\left(\frac{-\Delta E}{RT}\right) \tag{10}$$

where the equilibrium factor f_e is approximated as 1. The equilibrium constant for the shift reaction is expressed as

$$K_{\rm shift} = \exp\left(\frac{-\Delta G_{\rm wgs}}{RT}\right) \tag{11}$$

The change of Gibbs free energy is calculated by Eq. (3b). The reaction rates of the shift reaction are determined for both the forward and backward processes [13]

$$\eta_{\rm conc,c} = -\frac{RT}{4F} \ln \left(\frac{p_{\rm O_2}}{p_{\rm O_2}^e} \right) = -\frac{RT}{4F} \ln \left\{ \frac{(p_{\rm c}/\delta_{\rm O_2}) - \left[(p_{\rm c}/\delta_{\rm O_2}) - p_{\rm O_2}^e \right] \exp[(RT\delta_{\rm O_2}l_c|\vec{i}\cdot\vec{n}|)/(4FD_{\rm O_2(eff)}p_{\rm c})]}{p_{\rm O_2}^e} \right\}$$
(7)

where \vec{n} and l are shown in Fig. 2, and	$\dot{r}_{ m f} = k_1 x_{ m CO} x_{ m H_2O}$	(12a)
$\delta_{\rm O} = \frac{D_{\rm O_2, K(eff)}}{D_{\rm O_2, K(eff)}}$	$\dot{r}_{\mathrm{b}} = k_1 K_{\mathrm{shift}} x_{\mathrm{CO}_2} x_{\mathrm{H}_2}$	(12b)
$D_{O_2,K(eff)} + D_{O_2-N_2(eff)}$		

where k_1 is a constant.

2.3. Ohmic polarization

Ohmic losses, which arise from the resistance to charge conduction through the various cell components, depend linearly on current. Ohmic losses are due to electronic conduction of current occurring in the electrodes and the interconnector and ionic conduction of oxygen and anions through the solid electrolyte. The variation of the ohmic

3. Numerical method

The numerical simulation is performed using the CFD software, Fluent 6.1. Thermodynamic equations for the electrochemical reactions and governing equations are incorporated and solved by UDF. The standard $k - \varepsilon$ laminar model and SIMPLEC algorithm are used.



Fig. 2. A sketch of reaction gases diffusion in the electrode.

3.1. Governing equations

In each control volume, the governing differential equations, including continuity, momentum conservation, species transport, energy conservation and electric potential, are solved.

3.1.1. Conservation laws

The governing equations for steady fluid flow can be written as follows:

$$\operatorname{div}(\rho \vec{V}\phi) = \operatorname{div}(\Gamma_{\phi}\operatorname{grad}\phi) + S_{\phi} \tag{13}$$

where ϕ is a generic variable.

For the continuity equation, $\phi = 1$. For the other conservation equations, ϕ equals Y_i the mass fraction of each species for the transport equations, V_j the velocity for each direction for the momentum equations, T the temperature for the energy equation and Φ the electric potential for the charge equation. In the present model, we assume that the fluid has no effect on the conductivity of electric current. Then, for the electric potential equation,

$$\operatorname{div}(\rho V \Phi) = 0 \tag{14}$$

In Eq. (13), Γ_{ϕ} is the diffusion coefficient and S_{ϕ} is the source term for the generic variable ϕ . They are given in Ref. [14] for all conservation equations except the species transport equation and the electric potential equation. For the species transport equations, the dilute approximation is applied in laminar flow.

$$\Gamma_i = \rho D_{i,m} \tag{15a}$$

where $D_{i,m}$ is the diffusion coefficient for species *i* in the mixture. For the electric potential equation, we have

$$\Gamma_{\Phi} = \sigma \tag{15b}$$

3.1.2. Source terms

There are variations of heat and species concentrations due to the electrochemical reactions. In the presented model, these variations are incorporated into the source terms of the governing equations.

The volumetric heat source term s_q is the sum of the ohmic heat source, the chemical reaction heat and the radiant heat exchange. The discrete ordinates radiation model is applied to calculate the radiant heat exchange [15]. The ohmic heat is calculated by the following formulae:

$$Q_{\rm ohm} = \sigma {\rm grad} \Phi {\rm grad} \Phi \tag{16a}$$

For the control volume element in the anode side interlayer domain, the chemical reaction produced heat was calculated by the following equation:

$$Q_{\rm chem} = (\dot{r}_{\rm f} - \dot{r}_{\rm b})\Delta H_{\rm S} + \dot{r}_{\rm R}\Delta H_{\rm R} + \frac{|i \cdot \vec{n}|}{2F}A_{\rm CV}\Delta H_{\rm E}$$
(16b)

Elsewhere

$$Q_{\rm chem} = 0 \tag{16c}$$

So,

$$S_q = Q_{\rm ohm} + Q_{\rm chem} + Q_{\rm rad} \tag{16d}$$

The volumetric source terms for the species mass abide by the following equation:

$$S_{i} = M_{i}[k_{\mathrm{R},i}\dot{r}_{\mathrm{R}} + \kappa_{\mathrm{S},i}(\dot{r}_{\mathrm{f}} - \dot{r}_{\mathrm{b}}) + \kappa_{\mathrm{E},i}|\vec{i}\cdot\vec{n}|/(2F)A_{\mathrm{CV}}]$$
(17)

The volumetric reaction rates are calculated from Eqs. (10) and (12a), (12b).

Additionally, the porous media can be modeled by the addition of a momentum source term to the standard fluid flow equations. The source term consist of two parts, a viscous loss term and an inertial loss term. The equation is given as

$$S_{j} = -\left(\sum_{k=1}^{3} D_{j,k} \mu V_{k} + \sum_{k=1}^{3} \zeta_{j,k} \frac{1}{2} \rho |\vec{V}| V_{k}\right)$$
(18a)

where *j* denotes the *j*th (*x*, *y* or *z*) momentum equation, and *D* and ζ are prescribed matrices. In the present model, the porous medium is simply considered as homogenous. For the laminar model, the pressure drop is typically proportional to velocity, and the constant ζ can be considered to be zero. The porous media model then can be described by Darcy's Law

$$S_j = -\frac{\mu}{\alpha} V_j \tag{18b}$$

where $1/\alpha$ is a diagonal matrix to simply specify*D*.

3.2. Boundary conditions

The potential is continuous throughout the electric fields except for the electrolyte interfaces where the chemical reactions occur. Fig. 3 sketches the grid for computation of the local current density at the electrode/electrolyte interfaces. In Fig. 3, the ionic current density through the electrolyte is obtained by the following equation:



Fig. 3. The grid scheme for computation of current density at electrode/ electrolyte interfaces.

$$\vec{i} \cdot \vec{n} = \frac{E_{\rm n} - (\Phi_{P'} - \Phi_P)}{R_{\rm n}} \tag{19}$$

where R_n is the local lumped area specific electric resistance for the sum of polarization.

At the external boundary, the thermal flux and electric current flux are zero. Uniform potential is assumed, and the value is given at the current inlet and outlet. The temperature, the species mass fractions and the mass fluxes are imposed at the gas inlet. The pressure is given at the gas outlets.

4. Results

4.1. Validation of the model

In order to validate the model, two typical geometries of SOFC, a planar type and a tubular type, are calculated using the presented model.

4.1.1. Planar SOFC

The International Energy Agency (IEA) conducted a fuel cell stack modeling exercise involving seven European countries and Japan in 1995. Two cases of SOFC stack operation are simulated: (1) one cell stack operating with humidified hydrogen fuel and ambient air feed and (2) one cell stack operating with direct internal steam reforming of methane and air. These two cases were called in the IEA database "benchmark test 1" and "benchmark test 2", respectively. Since a simulation for the whole stack is time consuming, a simplified single unit cell model with bipolar channels is used in the present simulation. Furthermore, because the geometry of the single unit is symmetric, only half of the one repeating unit is simulated, which is illustrated in Fig. 4. The geometrical parameters for the calculation are given as follows: active area 2.71×100 mm, anode thickness 50 µm, cathode thickness 50 µm, electro-



Fig. 4. The calculation geometry of the half single-unit cell for the planar SOFC.

lyte thickness 150 μ m, channel height 1 mm, rib width 2.42 mm, and bipolar plate thickness 2.5 mm The permeability of the porous electrode is 1.0×10^{-8} /m² and its porosity is 0.2.

Numerical simulations are performed for two fuel composition cases with co-flow and counter-flow for a planar geometry. The operating condition parameters are described in Table 2. The laminar model is used. A symmetric boundary condition is applied at the symmetric surfaces. Current numerical results given in Table 3 are in agreement with the data of IEA. However, the current results for the maximal and minimal values of density are different from the IEA results. These differences are due to the effect caused by the electrode porous material. The porous material effect was not taken into account in the IEA test [16]. The gas molar fractions have a strong effect on the current density distribution. In the area underneath the interconnector rib, the gaseous species are transported only by diffusion in the porous electrodes. This leads to lower H₂ and higher H₂O molar fractions in the underneath interconnector rib area than in the channel area. This non-uniform distribution is more obvious when the porous material effect is considered in the present model. The lower H₂ molar fraction results in the lower current density. Thus, the obtained minimum value of current density is lower than that of IEA. The maximum current density is located in the channel area as shown in Fig. 5. For the counter-flow configuration, the distance between the maximum current density position and the fuel inlet is very short. So, the effect of the porous material on the gaseous

 Table 2

 Material properties and operating conditions for the planar SOFC [16]

	Cathode	Electrolyte	Anode	Interconnect
σ	$\frac{4.2 \times 10^7}{T} \exp\left(-\frac{1200}{T}\right)$	$3.34 \times 10^4 \exp\left(-\frac{10300}{T}\right)$	$\frac{9.5 \times 10^7}{T} \exp\left(-\frac{1150}{T}\right)$	$\frac{9.3 \times 10^6}{T} \exp\left(-\frac{1100}{T}\right)$
λ	3	2	3	3.5
Operating conditions				
Operating voltage (v)	Ca	se 1: co-flow 0.71, counter-flow 0.71 case	2: co-flow 0.65 counter-flow 0.69	
Operating pressure (bar)	1			
Inlet gas	117	3		
Temperature (K)				
Inlet gas	Ca	se 1: air: O ₂ 21%, N ₂ 79% fuel: H ₂ 90%, H	H ₂ O 10%	
Composition	Ca	se 2: air: O_2 21%, N_2 79% fuel: H_2 26.26%	6, H ₂ O 49.34%, CO 2.94%, CO ₂ 4	.36%, CH ₄ 17.10%

Table 3

Comparisons of the simulation results with benchmark test

	Case1 (co-flow/counter-flow)		Case2 (co-flow/coun	ter-flow)
	Benchmark	Present model	Benchmark	Present model
Voltage				
High	0.722/0.730	0.71/0.71	0.649/0.692	0.65/0.69
Low	0.702/0.709		0.633/0.680	
Average current density	3000/3000	2952/2964	3000/3000	2959/2931
Max current density				
High	3957/8970	4947/8246	3665/6554	4368/6402
Low	3725/7107		3040/5330	
Min current density				
High	1366/1235	390/631	2508/1332	637/722
Low	1020/1080		1748/994	
Max temperature				
High	1371/1357	1333/1339	1307/1362	1301/1326
Low	1321/1335		1294/1335	
Min temperature				
High	1203/1186	1184/1178	1135/1188	1139/1178
Low	1182/1177		1120/1179	
Fuel utilization	85%	83.6%/83.9%	85%	83.8%/83%

species molar fraction is very little at the maximum current density position. For the co-flow configuration, the distance between the maximum current density position and the fuel inlet is quite long, and the electrode porous material has a strong effect on the maximum current density



Fig. 5. The current density distribution through the electrolyte for the planar SOFC (case 2): (a) co-flow and (b) counter-flow.

because the distance is too long. The numerical result of the maximum current density value for the co-flow configuration is higher than that of the IEA test results.

4.1.2. Tubular SOFC

Fig. 6 shows the single tubular SOFC components configuration, which was designed by Siemens-Westinghouse Corporation. An injection tube in the interior of the cell is used to inject air to the active region of the cell. The electrolyte thickness is 40 µm. A 100 µm anode layer is attached on the electrolyte surface. The tubular SOFC is usually designed for the cathode support configuration. The cathode thickness is 2200 µm, which is larger than that of the electrolyte and anode. The electrode porosity is about 30-40%. At the bottom of the cell, there is the current collection component, which is named the interconnection. Its thickness equals 80 µm. The cell length is 1500 mm, and it has 834 cm^2 active areas. The cathode is continuous throughout the cylinder. The electrolyte acts through 312° of the circumference. It is interrupted by the interconnector on the top of the cell. The anode is also discontinuous, acting through a circumference of 288°, leaving the top open for



Fig. 6. The geometry of tubular SOFC components: (a) schematic configuration of a single cell for tubular SOFC and (b) cross section of the single tubular cell.

 Table 4

 The electrical conductivity of cell components for the tubular SOFC

Cell components	Electrical conductivity σ
Electrolyte	$3.401 \times 10^4 e^{-10350/T}$
Anode	$1.117 \times 10^7 e^{1392/T}$
Cathode	$1.232 \times 10^4 e^{-600/T}$
Interconnector	$3.981 \times 10^3 e^{-4690/T}$

electrical contact to the adjacent cell. Only half of the domain was calculated in this work because the unit cell geometry is a symmetrical configuration.

The operation temperature is about 1000 °C. Under this condition, the resistances for typical cells are 10 ohm cm (ionic) for the electrolyte (8–10 mol% Y₂O₃ doped ZrO₂), 1 ohm cm (electronic) for the cell interconnection (doped LaCrO₃), 0.01 ohm cm (electronic) for the cathode (doped LaMnO₃) and 3×10^{-6} ohm cm (electronic) for the anode (Li/CrO₂ cermets). Apparently, the solid oxide fuel cell electrolyte is the least conductive of the cell components, followed by the interconnection. The conduction of the cell components is shown in Table 4. In this paper, the constants of the expo-



Fig. 7. Comparison of the performance of present model predictions and experiment data for the tubular SOFC.



Fig. 8. Temperature contour on the electrolyte surface (average current density $= 3100 \text{ A/m}^2$).

nent were selected from Ref. [1], and the coefficients are determined based on Ref. [17].

The fuel consists of a mixture of 89% molar H_2 and 11% molar H_2O . The air used in the simulation is six times more than the stoichiometric requirement. The inlet air and fuel temperatures are set to be 873 K and 1123 K, respectively. The simulations are conducted in atmospheric pressure with a varied output voltage. Fig. 7 shows the comparison of the present simulation results and the Siemens Westinghouse test data [17]. The numerical results are in good agreement with the test data.

Fig. 8 shows the temperature distribution on the electrolyte surface. In the middle area, the electrolyte temperature rises along the gas flow direction because of the exothermic electrochemical reaction. Downstream of the gas steam, the electrolyte temperature decreases along the gas steam, since the electrolyte is cooled by the incoming lower temperature air.

The changes of the gaseous molar fraction on the electrolyte surface are shown in Fig. 9. The reacting gases, H_2 and O_2 , decrease along the gas flow direction, and the



Gas flow

Fig. 9. Gases molar fraction contour on the electrolyte surface (average current density = 3100 A/m^2): (a) H₂ molar fraction contour, (b) H₂O molar fraction contour and (c) O₂ molar faction contour.

molar fraction of the product gas H_2O increases with the electrochemical reaction along the gases flow direction. The electrolyte and the anode are not continuous through the circumference because of the connector on the electrode. It causes the concentration difference through the circumference.

4.2. Analysis of electric characteristics

Fig. 10 shows the electric potential and current density vector at the section z = L/2 for the planar and tubular geometries, respectively. The electric potential decreases along the current flow due to the ohmic resistance as shown in Fig. 10. For the planar SOFC, both the current density and the output voltage within the channel area



Fig. 10. The contour of electric potential and the vector of current density (z = L/2): (a) planar (case 2 co-flow) and (b) tubular (average current density = 3100 A/m²).

are higher than those underneath the interconnector rib area. However, for the tubular configuration, only the anode current density is higher than the cathode current density due to its thin thickness. At the anode side, the current density decreases along the current flow because the current flows through the electrolyte from the anode to the cathode. At the cathode side, the current density increases along the current flow. The cathode ohmic loss is very high compared with that of the electrode and interconnector. Additionally, the ohmic loss of the interconnector is large due to its high current density.

Fig. 11 shows the polarization losses for the two configurations of SOFC. The angle direction for the tubular SOFC is shown in Fig. 10(b). As Fig. 11(a) shows, the maximal polarization loss comes from the electrolyte ohmic loss because the electrolyte thickness of the planar SOFC is higher than that of the electrodes, and the electrolyte conductivity is the least among the electric components. For the tubular SOFC, the maximal loss is contributed by the cathode ohmic loss due to its high electric resistance and very long path for the current flow. The anode ohmic loss can be almost neglected because



Fig. 11. Polarization for the SOFCs (z = L/2): (a) planar (case 2 co-flow) and (b) tubular (average current density = 3100 A/m²).

of its very small electric resistance even though its current density is quite high.

The following maximal polarization is an active loss of both the planar and tubular configurations. The sum of the average anode and cathode active polarization contributes about 55% for the planar configuration and 30% for the tubular configuration in the total polarization losses. As indicated by Eq. (5a), the exchange current density is the key element that affects the active polarization. A high exchange current density is pursued in order to decrease the active polarization. However, the exchange current density depends on the material property, the production technology and the partial pressures of the reaction species. The anode concentration polarization is very small according to Fig. 11.

Fig. 12 is the output voltage between the anode and cathode in the planar SOFC. The current density distribution through the electrolyte of the planar SOFC is shown in Fig. 5. Within the channel area, both the output voltage and current density are much higher than those underneath the interconnector rib area. The maximal value position of the co-flow configuration appears later than that of the counter-flow configuration in the fuel flow direction. These characteristics are caused by the different species concen-



Fig. 12. The output voltage between anode and cathode for the planar SOFC (case 2).

trations at the reaction site. Underneath the interconnector rib, the reactive gases species are transported by diffusion through the porous electrode. Therefore, the reactive species concentration is lower and the resultant species concentration is higher compared to that of the channel area. The Enerst potential, which determines the output of voltage, in the channel area is higher than that underneath the interconnector rib area. Additionally, the current density for the counter-flow configuration is less uniformly distributed than that of the co-flow configuration as shown in Fig. 5.

Fig. 13 shows the current flow in the gas flow direction for the planar SOFC. As can be seen from the plotted results, the current flow exhibits three dimensional characteristics, especially at the electrode. At the anode side, the current converges to the middle in the z axial direction. The opposite appears at the cathode side. These characteristics are in agreement with the gradients of potential in the electric components, which are shown in Fig. 14. In the middle of z axial area, the potential is lower in the anode side and higher in the cathode side. Then, the current flows from the high potential area to the low potential area in the z axial direction.

Fig. 15 shows the generated heat from the ohmic resistance for the planar and tubular configurations, respectively. For the planar SOFC, only the anode side electric components of the case 2 co-flow configuration are shown in Fig. 15(a). The cathode side is not presented here as it has a similar distribution. Within the electrode domain of the planar SOFC, as shown in Fig. 15(a) and Fig. 10(a), the generated ohmic heat is much higher than that in the interconnector due to the higher current density. For the tubular SOFC, as shown in Fig. 15(b), most of the ohmic heat is generated within the cathode due to its lower electric conductivity. The total ohmic heat from all components is given in Table 5 for both the planar and tubular SOFC. The calculated results show that the contribution of ohmic heat in the



Fig. 13. Contours of current density vector in the z direction: (a) anode, (b) anode side connector, (c) cathode and (d) cathode side connector.



Fig. 14. Contours distribution of potential: (a) anode side and (b) cathode side.



Fig. 15. The generated heat for ohmic resistance (anode side): (a) planar (anode side for case 2 co-flow) and (b) tubular (average current density = 3100 A/m^2).

Table 5					
The sum of	generated	ohmic	heat in	the SOFC	

	Planar					
	Case 1 (co-flow/c	ounter-flow)	Case 2 (co-flow/c	ounter-flow)		
Ohmic heat (W)	0.0108063	0.013946	0.0099785	0.0120456	6.77999	
Total generated heat (w)	0.4552267	0.4689177	0.3311145	0.2940901	84.84166	
$Q_{\rm ohm}/Q_{\rm tot}$	2.37%	2.97%	3%	4.1%	8%	

total generated heat for the tubular configuration is greater than that of the planar configuration. For the planar SOFC, the percents of ohmic heat in the total generated heat for the counter-flow is greater than that of the co-flow configuration.

5. Conclusions

A three dimensional complete polarization model for the solid oxide fuel cell is developed in this paper. The internal reforming process and the water-gas shift reaction have been taken into account in the model. Numerical simulations are performed for both planar and tubular geometry SOFCs. Current simulation results have been compared with the results from other simulations for the planar geometry and experimental data. The comparisons show that the present model is accurate in predicting the behavior of the SOFC with various geometries.

In the planar SOFC, the polarizations mostly come from the electrolyte ohmic loss and the active polarization. For the tubular SOFC, the cathode ohmic loss is the greatest contribution to the sum of polarizations, while the active polarization is the second highest loss. At the anode side, the current flow converges to the middle site where the potential is lower compared to the cathode side where the current flow trend is opposite to that of the anode side. The ohmic heat mainly depends on the current density in the planar configuration. In the tubular SOFC, mostly the ohmic heat is produced from the cathode. The relative ohmic heat contribution to the total heat is higher for the tubular than for the planar configuration, and this is more pronounced in the counter-flow design than in the co-flow design for the planar SOFC.

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