

One-dimensional Dynamic Modeling and Simulation of a Planar Direct Internal Reforming Solid Oxide Fuel Cell^{*}

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Abstract This article aims to investigate the transient behavior of a planar direct internal reforming solid oxide fuel cell (DIR-SOFC) comprehensively. A one-dimensional dynamic model of a planar DIR-SOFC is first developed based on mass and energy balances, and electrochemical principles. Further, a solution strategy is presented to solve the model, and the International Energy Agency (IEA) benchmark test is used to validate the model. Then, through model-based simulations, the steady-state performance of a co-flow planar DIR-SOFC under specified initial operating conditions and its dynamic response to introduced operating parameter disturbances are studied. The dynamic responses of important SOFC variables, such as cell temperature, current density, and cell voltage are all investigated when the SOFC is subjected to the step-changes in various operating parameters including both the load current and the inlet fuel and air flow rates. The results indicate that the rapid dynamics of the current density and the cell voltage are mainly influenced by the gas composition, particularly the H₂ molar fraction in anode gas channels, while their slow dynamics are both dominated by the SOLID (including the PEN and interconnects) temperature. As the load current increases, the SOLID temperature and the maximum SOLID temperature gradient both increase, and thereby, the cell breakdown is apt to occur because of excessive thermal stresses. Changing the inlet fuel flow rate might lead to the change in the anode gas composition and the consequent change in the current density distribution and cell voltage. The inlet air flow rate has a great impact on the cell temperature distribution along the cell, and thus, is a suitable manipulated variable to control the cell temperature.

Keywords solid oxide fuel cell, direct internal reforming, planar, dynamic model, simulation

1 INTRODUCTION

The solid oxide fuel cell (SOFC) is attracting more and more interests as a clean and highly efficient device for power generation [1]. Since it uses an oxide ceramic material as the electrolyte, high operating temperature (typically 600–1000°C) is required to achieve sufficient ionic conductivity. The high temperature makes it possible that the fuel reforming, when a hydrocarbon is used as the fuel, is carried out directly within the anode channels, giving rise to a direct internal reforming SOFC (DIR-SOFC) [1]. The direct internal reforming eliminates the need for a separate fuel reformer, and can lead to a more compact and efficient system design. In addition, the high operating temperature also produces high quality waste heat, which can be recycled by heat recovery devices or gas turbines to make combined heat and power (CHP) or hybrid systems with very high overall efficiency.

As an SOFC system in operation is normally subjected to frequent load changes, it's crucial to investigate the dynamic behavior of an SOFC caused by variable load or other operating parameters. Dynamic modeling is a valid tool for predicting the dynamic behavior of the SOFC. Through model-based dynamic simulations, some dynamic features of the SOFC can be revealed and control strategies can furthermore be developed. Up to now, a number of SOFC models can be found in the published works. Although most of

them describe SOFC steady-state performance [2–5], dynamic issues have also been addressed by several authors. Hall and Colclaser [6], and Xue *et al.* [7] developed one-dimensional dynamic models to analyze the transient behavior of tubular SOFCs. However, the internal reforming effect was not included in their models. Achenbach *et al.* [8, 9] presented a three-dimensional dynamic model for a planar SOFC with inclusion of the internal reforming effect and examined the transient cell voltage response to load changes as well as the influence of several design parameters on the transient performance. However, the transient current density response of the SOFC is not yet well known. Aguiar *et al.* [10, 11] proposed a one-dimensional dynamic model for a planar DIR-SOFC, by which the steady and dynamic performance of the SOFC was investigated. However, in their model, some gas properties, such as gas densities, heat capacities and velocities, were taken as constant values. Moreover, besides the response to load changes, none of the above authors considers the transient behavior caused by changes in other operating parameters (*e.g.*, the inlet fuel and air flow rates), which can give insight into the effects of these operating parameters and benefit developing appropriate control strategies.

The main objective of this article is to investigate the transient behavior of a planar DIR-SOFC more comprehensively. In this article, the dynamic responses of important SOFC variables, such as cell

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temperature, current density, and cell voltage, will all be considered when the SOFC is subjected to the changes in various operating parameters including both the load and the inlet fuel and air flow rates. The authors, here, try to provide a clear picture of these variables as functions of position and time. For this purpose, a one-dimensional dynamic model of a planar DIR-SOFC is first developed based on mass and energy balances, and electrochemical principles. Furthermore, a solution strategy is presented and a MATLAB code is designed to solve the model. Next, the International Energy Agency (IEA) benchmark test [12] is used to validate the present model. Then, through model-based simulations, the steady-state performance of a co-flow planar DIR-SOFC under specified initial operating conditions, and its dynamic response to introduced operating parameter disturbances are investigated in detail.

2 MODEL DEVELOPMENT

Figure 1 shows the schematic diagram of a unit planar DIR-SOFC. Its core component is a tri-layer structure (often referred to as the PEN) consisting of two porous electrodes, anode and cathode, separated by a dense ion-conducting electrolyte. Two interconnect plates with machined gas channels are placed above and below the PEN to form a unit cell. To compose an SOFC stack, repeating unit cells need to be further connected in series. The methane mixed with water steam (or their product after pre-reforming of some degree) is usually used as fuel at the anode side, and air is used as an oxidant at the cathode side.

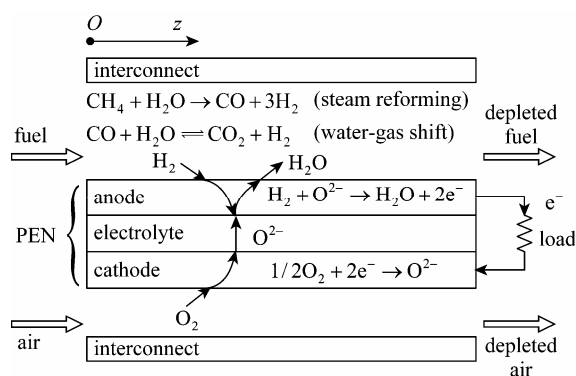


Figure 1 Schematic diagram of a unit planar DIR-SOFC

Because of the high temperature in anode channels, the methane is reformed to H_2 , CO , and CO_2 directly on the anode mainly through two reactions, *i.e.*, the methane steam reforming and the water-gas shift (WGS). The H_2 , which is produced, is then electrochemically oxidized by oxygen ions that migrate through the electrolyte from the cathode side, producing water and heat, and releasing electrons. The released electrons drive the external load to perform electrical work and return to the cathode, where they electrochemically reduce the O_2 to oxygen ions. All the reactions taken into account in the present model are listed in Table 1. Although the electrochemical oxidation of CO also occurs on the anode, it is neglected, here, because its speed is 2–5 times slower than that of H_2 oxidation [12, 13].

For model development, several assumptions are made as follows:

(1) Each unit cell in the SOFC stack operates identically, and there is no heat transfer between adjacent unit cells. Therefore, a unit cell can be investigated to represent the full stack performance.

(2) The SOFC is treated as a one-dimensional plant along the gas flow direction. Therefore, this model allows for the co-flow and counter-flow rather than cross-flow configuration although the equations presented next are for the co-flow case. Correspondingly, a one-dimensional coordinate system is built with its coordinate origin located at the anode channel inlet and the forward direction of z -axis along the fuel flow direction (see also Fig. 1).

(3) The SOFC is divided into three temperature layers, *i.e.*, the fuel stream in the anode channels (T_a), the air stream in the cathode channels (T_c), and the solid part (T_s), where the solid part (also referred to as SOLID in this article) includes both the PEN and the interconnects, *i.e.*, $T_s = T_{PEN} = T_{int}$.

(4) All gases are assumed to be ideal gas.

(5) The pressure in the gas channels is assumed to be constant.

2.1 Mass balances

According to the reactions listed in Table 1, there are five gas species in the anode channels, *i.e.*, CH_4 , H_2O , H_2 , CO , and CO_2 , and two gas species in the cathode channels, *i.e.*, O_2 and N_2 . By applying the molar balance to species i in the anode channels, the following equation is obtained:

Table 1 Reactions considered in the model

No.	Reaction name	Reaction equation	$\Delta H/J \cdot mol^{-1}$
(i)	methane steam reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$	206100
(ii)	water-gas shift	$CO + H_2O \rightleftharpoons CO_2 + H_2$	-41150
(iii)	hydrogen oxidation	$H_2 + O^{2-} \rightarrow H_2O + 2e^-$	-
(iv)	oxygen reduction	$1/2 O_2 + 2e^- \rightarrow O^{2-}$	-
(v)	overall electrochemical reaction	$H_2 + 1/2 O_2 \rightarrow H_2O$	241800

$$\frac{\partial(C_a x_{i,a})}{\partial t} + \frac{1}{A_a} \frac{\partial(N_a x_{i,a})}{\partial z} = S_{m,i,a},$$

$$i \in \{\text{CH}_4, \text{H}_2\text{O}, \text{H}_2, \text{CO}, \text{CO}_2\}, \quad (1)$$

where C_a is the total molar concentration of anode gases, $x_{i,a}$ the molar fraction of species i in the anode gas stream, A_a the total sectional area of anode channels, N_a the molar flow rate of the anode gas stream, and $S_{m,i,a}$ the mass source term of species i in anode channels.

For the gases in the anode channels, the following total molar balance equation can also be built:

$$\frac{\partial C_a}{\partial t} + \frac{1}{A_a} \frac{\partial N_a}{\partial z} = S_{m,a}, \quad (2)$$

where $S_{m,a}$ is the total mass source term of the gases in the anode channels.

Insertion of Eq. (2) into Eq. (1) yields the following molar fraction dynamic equation of species i in the anode channels:

$$C_a \frac{\partial x_{i,a}}{\partial t} + \frac{1}{A_a} \frac{\partial(N_a x_{i,a})}{\partial z} = \frac{x_{i,a}}{A_a} \frac{\partial N_a}{\partial z} + S_{m,i,a} - x_{i,a} S_{m,a}. \quad (3)$$

Plugging the ideal gas law $C_a = p_a / (RT_a)$ into Eq. (2) and applying the constant pressure assumption [*i.e.*, Assumption (5)] result in the following temperature dynamic equation of anode gas phase:

$$-\frac{p_a}{RT_a^2} \frac{\partial T_a}{\partial t} + \frac{1}{A_a} \frac{\partial N_a}{\partial z} = S_{m,a}, \quad (4)$$

where p_a is the pressure in the anode channels, T_a is the temperature of anode gas phase, and R is the universal gas constant.

Similarly, the molar fraction dynamic equation and temperature dynamic equation for cathode gases can also be derived as follows:

$$C_c \frac{\partial x_{i,c}}{\partial t} + \frac{1}{A_c} \frac{\partial(N_c x_{i,c})}{\partial z} = \frac{x_{i,c}}{A_c} \frac{\partial N_c}{\partial z} + S_{m,i,c} - x_{i,c} S_{m,c},$$

$$i \in \{\text{O}_2, \text{N}_2\}, \quad (5)$$

$$-\frac{p_c}{RT_c^2} \frac{\partial T_c}{\partial t} + \frac{1}{A_c} \frac{\partial N_c}{\partial z} = S_{m,c}. \quad (6)$$

The mass source terms of individual gas species, *i.e.*, $S_{m,i,a}$ and $S_{m,i,c}$, and the total mass source terms, *i.e.*, $S_{m,a}$ and $S_{m,c}$, are related to the rates of reactions in the SOFC. Defining a vector $\mathbf{r} = [r_i \ r_{ii} \ r_{iii} \ r_{iv}]^T$ to represent the rates of reactions (i)–(iv), these mass source terms can be expressed as:

$$S_{m,i,k} = \mathbf{a}_{i,k}^T \text{diag}(W/A_a, W/A_a, W/A_a, W/A_c) \mathbf{r}, \quad (7)$$

and

$$S_{m,k} = \mathbf{a}_k^T \text{diag}(W/A_a, W/A_a, W/A_a, W/A_c) \mathbf{r},$$

$$k \in \{a, c\}, \quad (8)$$

where $\mathbf{a}_{i,k} \in R^4$ is the stoichiometric vector of species i in gas stream k in reactions (i)–(iv), $\mathbf{a}_k \in R^4$ is the total stoichiometric vector of gas stream k in reactions (i)–(iv), and W is the cell width. Obviously, there exists the following relation between the two types of stoichiometric vectors:

$$\mathbf{a}_k = \sum_{i=1}^{\zeta_k} \mathbf{a}_{i,k}, \quad (9)$$

where ζ_k is the number of gas species with $\zeta_a = 5$ for the anode gas stream and $\zeta_c = 2$ for the cathode case.

The reaction rate of the steam reforming is calculated by the following equation [8, 10, 14]:

$$r_i = k_r p_a x_{\text{CH}_4,a} \exp\left(-\frac{E_{A,r}}{RT_a}\right), \quad (10)$$

with $k_r = 0.04274 \text{ mol} \cdot \text{s}^{-1} \cdot \text{m}^{-2} \cdot \text{Pa}^{-1}$ and $E_{A,r} = 82000 \text{ J} \cdot \text{mol}^{-1}$, where k_r is the pre-exponential constant and $E_{A,r}$ is the activation energy of the steam reforming reaction.

The WGS reaction is usually considered a very fast one and is assumed to be at its equilibrium. The formula proposed by Aguiar *et al.* [10] is used here to account for this effect:

$$r_{ii} = k_{sh} p_a x_{\text{CO},a} \left[1 - \frac{x_{\text{CO}_2,a} x_{\text{H}_2,a} / (x_{\text{CO},a} x_{\text{H}_2\text{O},a})}{K_{sh}} \right], \quad (11)$$

where $k_{sh} = 0.01$ in this model and K_{sh} is the equilibrium constant with $K_{sh} = \exp(4276/T_a - 3.961)$ [15].

According to the charge conservation, the reactions (iii)–(v) have the same reaction rate, which is related to the local current density j and can be calculated by Faraday's law:

$$r_{iii} = r_{iv} = r_v = \frac{j}{2F}. \quad (12)$$

The boundary conditions of Eqs. (3)–(6) are specified by the inlet gas conditions. For the co-flow configuration, they can be written as follows:

$$x_{i,a}|_{z=0} = x_{i,a}^0, \quad N_a|_{z=0} = N_a^0, \quad x_{i,c}|_{z=0} = x_{i,c}^0,$$

$$N_c|_{z=0} = N_c^0. \quad (13)$$

2.2 Energy balances

According to Assumption (3), the energy balance is applied to the gas phase in the anode and cathode channels, and the SOLID, respectively. The energy balance for the anode gas phase can be written as:

$$\frac{\partial(C_a h_a)}{\partial t} + \frac{1}{A_a} \frac{\partial(N_a h_a)}{\partial z} = S_{h,a}, \quad (14)$$

where h_a is the molar specific enthalpy of the anode gas mixture, and $S_{h,a}$ is the heat source term for the anode gas phase. If h_a is roughly considered to be a linear function of temperature, the first term on the left hand side of Eq. (14), which represents the energy

accumulation in the gas phase, becomes zero by inserting the ideal gas law into it and applying the constant pressure assumption. Therefore, this term can be neglected and the following ordinary differential equation is obtained:

$$\frac{1}{A_a} \frac{\partial(N_a h_a)}{\partial z} = S_{h,a} \quad (15)$$

Similarly, for the cathode gas phase, we can obtain:

$$\frac{1}{A_c} \frac{\partial(N_c h_c)}{\partial z} = S_{h,c} \quad (16)$$

The energy balance equation for the SOLID can be written as:

$$\frac{\partial(\rho_s c_{p,s} T_s)}{\partial t} = \lambda_s \frac{\partial^2 T_s}{\partial z^2} + S_{h,s} \quad (17)$$

where ρ_s , $c_{p,s}$, T_s , λ_s , and $S_{h,s}$ denote the density, mass specific heat capacity, temperature, thermal conductivity, and heat source term of the SOLID, respectively. As there is no macroscopic flow for the SOLID, the diffusion term rather than the convection term is included in this equation.

The heat source terms $S_{h,a}$, $S_{h,c}$, and $S_{h,s}$ are given by:

$$S_{h,a} = [l_{s,a} k_{s,a} \cdot (T_s - T_a) - W r_{iii} \cdot h_{H_2}(T_a) + W r_{iii} \cdot h_{H_2O}(T_s) - W r_i \Delta H_i - W r_{ii} \Delta H_{ii}] / A_a \quad (18)$$

$$S_{h,c} = [l_{s,c} k_{s,c} \cdot (T_s - T_c) - (W r_{iv} / 2) \cdot h_{O_2}(T_c)] / A_c \quad (19)$$

$$S_{h,s} = [-l_{s,a} k_{s,a} \cdot (T_s - T_a) - l_{s,c} k_{s,c} \cdot (T_s - T_c) + W r_{iii} \cdot h_{H_2}(T_a) + (W r_{iv} / 2) \cdot h_{O_2}(T_c) - W r_{iii} \cdot h_{H_2O}(T_s) - W r_v \Delta H_v - W U j] / A_s \quad (20)$$

where $l_{s,a}$ ($l_{s,c}$) denotes the total sectional perimeter of the anode (cathode) channels, $k_{s,a}$ ($k_{s,c}$) is the convective heat transfer coefficient between the anode (cathode) channels and the SOLID, $h_i(T)$ is the specific enthalpy of gas species i at the temperature of T , ΔH_j is the enthalpy change of reaction j at the temperature of 298.15 K, U is the SOFC operating voltage, and A_s is the sectional area of the SOLID.

In the above energy balances [Eqs. (15)–(20)], the heat conduction in the SOLID, the enthalpy flux because of the convection in the gas flow direction, the convective heat transfer between the gas channels and the SOLID, the enthalpy flux associated with the gas diffusion (*i.e.*, the reactive H_2 and O_2 enter the SOLID and the produced H_2O leaves the SOLID), and the heat release or absorption of the reactions are all considered. The heat conduction is modeled by Fourier's law. The convective heat transfer coefficient between the gas channels and the SOLID is calculated using a constant Nusselt number, which is taken to be 3.09 in this article [10, 16]. The diffusion rates of H_2 , O_2 , and H_2O are assumed to be equal to their reaction or production rates in the electrochemical reactions.

The specific enthalpy of gas species i at the temperature of T , $h_i(T)$, is calculated by:

$$h_i(T) = \int_{T^{ref}}^T c_{p,i}(T) dT \quad (21)$$

with $T^{ref} = 298.15$ K, where $c_{p,i}$ is the molar specific heat capacity of species i and is expressed as a third degree polynomial function of T [17]. The specific enthalpy of the gas mixture [*e.g.*, h_a and h_c in Eqs. (15) and (16)] is calculated as a function of the local gas molar fraction by

$$h_k = \sum_{i=1}^{\zeta_k} x_{i,k} h_i, \quad k \in \{a, c\} \quad (22)$$

The boundary conditions of Eqs. (15) and (16) are also specified by the inlet gas conditions. For the co-flow configuration, they can be written as follows:

$$\begin{aligned} T_a|_{z=0} &= T_a^0, \quad x_{i,a}|_{z=0} = x_{i,a}^0, \quad N_a|_{z=0} = N_a^0, \\ T_c|_{z=0} &= T_c^0, \quad x_{i,c}|_{z=0} = x_{i,c}^0, \quad N_c|_{z=0} = N_c^0. \end{aligned} \quad (23)$$

The two ends of the SOLID are both assumed to be insulated. Therefore, the boundary conditions of Eq. (17) are given as insulation conditions:

$$\left. \frac{\partial T_s}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial T_s}{\partial z} \right|_{z=L} = 0 \quad (24)$$

where L is the cell length.

2.3 Electrochemical model

The electrochemical model is used to calculate the cell operating voltage and the current density distribution. The operating voltage of the SOFC is generically given by subtracting three kinds of overpotential losses, *i.e.*, ohmic, activation, and concentration overpotentials from the reversible open circuit voltage as the following equation:

$$U = U_{OCV} - \eta_{ohm} - \eta_{act} - \eta_{conc} \quad (25)$$

As both the electrodes and interconnects are normally good conductors, a constant operating voltage throughout the cell is considered (*i.e.*, the electrodes and interconnects are considered as an equipotential surface), whereas the reversible open circuit voltage and various overpotentials are all local quantities, which depend on the local cell temperature, gas molar fractions, and current density, and will be explained next. To determine the cell operating voltage and the current density distribution, the average current density, which reflects the external load demand, also needs to be specified. The average current density is the average value of the local current density along the cell length and is defined by:

$$J = \frac{1}{L} \int_0^L j dz \quad (26)$$

The reversible open circuit voltage, U_{OCV} , is determined by the Nernst equation:

$$U_{OCV} = U_0(T_s) + \frac{RT_s}{2F} \ln \left[\frac{x_{H_2,a} x_{O_2,c}^{0.5} (p_c / p^{ref})^{0.5}}{x_{H_2O,a}} \right] \quad (27)$$

with $U_0(T_s) = 1.2723 - 2.7645 \times 10^{-4} T_s$, where $U_0(T_s)$ is the reversible open circuit voltage at the temperature of T_s and standard pressure [15].

The ohmic overpotential, η_{ohm} , is because of the electronic and ionic resistance along the path of the current in the fuel cell, and is determined by the Ohm's law as:

$$\eta_{\text{ohm}} = jR_{\text{ohm}}, \quad (28)$$

where R_{ohm} is the internal resistance of the cell and is calculated from the conductivity of the individual layers [10] by

$$R_{\text{ohm}} = \frac{\tau_a}{\sigma_a} + \frac{\tau_{\text{el}}}{\sigma_{\text{el}}} + \frac{\tau_c}{\sigma_c}. \quad (29)$$

The activation overpotential, η_{act} , is because of the energy barriers to be overcome so that the electrochemical reaction can occur and is calculated by the following equation [18]:

$$\eta_{\text{act}} = \frac{RT_s}{n_e F} \sinh^{-1} \left(\frac{j}{2j_{0,a}} \right) + \frac{RT_s}{n_e F} \sinh^{-1} \left(\frac{j}{2j_{0,c}} \right), \quad (30)$$

where n_e is the number of electrons transferred per electrochemical reaction ($n_e = 2$), and $j_{0,a}$ ($j_{0,c}$) is the anodic (cathodic) exchange current density. The exchange current densities are modeled in the following form [19]:

$$j_{0,a} = \beta_a \left(\frac{p_a x_{\text{H}_2,a}}{p^{\text{ref}}} \right) \left(\frac{p_a x_{\text{H}_2\text{O},a}}{p^{\text{ref}}} \right)^{-0.5} \exp \left(-\frac{E_{A,a}}{RT_s} \right), \quad (31)$$

$$j_{0,c} = \beta_c \left(\frac{p_c x_{\text{O}_2,c}}{p^{\text{ref}}} \right)^{0.25} \exp \left(-\frac{E_{A,c}}{RT_s} \right). \quad (32)$$

The concentration overpotential, η_{conc} , is because of the change in the reactant and product concentration at the reaction site as the bulk flow in gas channels, which results from the insufficient rate of gas diffusion in the porous electrode. Herein, it is modeled by a simple formula [20]:

$$\eta_{\text{conc}} = -\frac{RT_s}{n_e F} \ln \left(1 - \frac{j}{j_L} \right), \quad (33)$$

where j_L is the limiting current density, at which the fuel is used up at a rate equal to its maximum supply speed.

3 SOLUTION METHOD

The Eqs. (3)–(8), (10)–(13), and (15)–(33) introduced above compose the SOFC model, which is an equation system consisting of a set of partial differential equations, ordinary differential equations, algebraic equations, and relevant boundary conditions. Once the average current density, the inlet gas conditions (including the inlet molar flow rates, molar fractions, and temperatures of the anode and cathode gas streams), and the initial conditions (including the ini-

tial molar fraction distribution of each gas species, and the initial temperature distributions of the anode and cathode gas streams and the SOLID) are specified, it can be solved using the numerical method [21, 22].

The SOFC domain is divided into n uniform nodes along the cell length direction, with the grid points located at the centers of the nodes. The convection terms in the equation system are discretized using the first-order upwind scheme and the diffusion terms using the second-order central difference scheme. As the equation system is stiff, its transient terms are integrated using the stiff solver ode23s provided by MATLAB R2006a. In each time step, according to the specified average current density, the electrochemical model is first solved to obtain the cell voltage and the current density distribution through the use of the Newton-Raphson iteration. Afterwards, the mass source terms [Eqs. (7) and (8)] and heat source terms [Eqs. (18)–(20)] are calculated. Next, the molar flow rates, N_a and N_c , are calculated from Eqs. (15) and (16). Then, the state variables are updated from Eqs. (3)–(6) and (17). According to the solution strategy presented, a MATLAB code is designed to solve this model.

4 MODEL VALIDATION

The present SOFC model is validated by comparing its performance predictions with the results of the IEA benchmark test [12]. The benchmark test is a fuel cell stack modeling exercise conducted by IEA in 1995, which involves seven European countries and Japan. The simulated case used here for the model validation is a unit planar electrolyte-supported DIR-SOFC with co-flow configuration. The dimensions of the unit cell are given as follows: active area 100 mm×100 mm, anode thickness 50 μm , cathode thickness 50 μm , electrolyte thickness 150 μm , interconnect plate thickness 2.5 mm, number of channels 18, channel height 1 mm, channel width 3 mm, and rib width 2.42 mm. The input parameters of the benchmark test are listed in Table 2. To avoid discrepancies caused by different treatment of the electrochemical kinetics, the anodic and cathodic overpotentials (including the activation and concentration overpotentials) are regarded as being of the same amount as the ohmic loss of the electrolyte.

The comparison of the present model predictions and the IEA benchmark test results are given in Table 3. "High" and "low" in the table refer to the highest and lowest values reported by the participants of the IEA benchmark test. It can be found that in all compared items the present model predictions fall quite close to or lie between the high and low values of the IEA benchmark test. The cell voltage predicted by the present model is slightly higher than the IEA values (the voltage deviation is less than 3.5%). This is partly because of the negligence of the ohmic loss of interconnects. The good agreement between the present model predictions and the IEA benchmark results demonstrates the effectiveness of the present model.

Table 2 Parameters used in model validation [12]

	Parameter	Value
material properties of the cell	anode electrical conductivity/ $\Omega^{-1}\cdot\text{m}^{-1}$	$(9.5\times 10^7/T)\exp(-1150/T)$
	cathode electrical conductivity/ $\Omega^{-1}\cdot\text{m}^{-1}$	$(4.2\times 10^7/T)\exp(-1200/T)$
	electrolyte ionic conductivity/ $\Omega^{-1}\cdot\text{m}^{-1}$	$3.34\times 10^4\exp(-10300/T)$
	density/ $\text{kg}\cdot\text{m}^{-3}$	6600
	heat capacity/ $\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	400
	thermal conductivity/ $\text{J}\cdot\text{s}^{-1}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	2
operating conditions	average current density/ $\text{A}\cdot\text{m}^{-2}$	3000
	fuel utilization	0.85
	air ratio	7
	pressure/Pa	1.0×10^5
	inlet fuel temperature/K	1173
	inlet air temperature/K	1173
	inlet fuel composition	$\text{CH}_4 : 0.171, \text{H}_2\text{O} : 0.4934, \text{H}_2 : 0.2626, \text{CO} : 0.0294, \text{CO}_2 : 0.0436$
	inlet air composition	$\text{O}_2 : 0.21, \text{N}_2 : 0.79$

Table 3 Results of model validation

		Cell voltage/V	Power/W	Max. current density/ $\text{A}\cdot\text{m}^{-2}$	Min. current density/ $\text{A}\cdot\text{m}^{-2}$	Max. solid temperature/K	Min. solid temperature/K
IEA benchmark [12]	high	0.649	19.47	3665	2508	1307	1135
	low	0.633	18.99	3040	1748	1294	1120
the present model		0.6617	19.85	3588	1983	1309	1125

5 SIMULATION RESULTS AND DISCUSSION

The present model is able to predict some SOFC variables, including the cell temperature, the gas molar fractions, the cell voltage and the current density, along the cell length as well as their variation with time. Using this model, simulations are performed to investigate the behavior of a co-flow planar anode-supported intermediate-temperature DIR-SOFC. Parameters used in the simulations are listed in Table 4. The activation energy and limiting current density are typical values for anode-supported intermediate-temperature SOFCs. The anodic and cathodic pre-exponential coefficients are determined to guarantee reasonable activation overpotentials. Here, the anode area specific resistance of not more than $1.0\times 10^{-5} \Omega\cdot\text{m}^2$ and the cathode one of around $2\times 10^{-5} \Omega\cdot\text{m}^2$ at 1073 K are considered reasonable for anode-supported intermediate-temperature SOFCs [10, 18]. For the initial operating conditions, the average current density value is chosen to make the cell operate at a voltage between 0.6 and 0.7 V. The air ratio value guarantees a temperature increase along the cell of around 100 K. The inlet fuel has a steam/carbon ratio above 2 to avoid the occurrence of carbon deposition. In this section, the steady-state performance of the cell for the initial operating conditions is first presented. Then, its transient behavior is analyzed when some operating parameter disturbances are imposed.

5.1 Steady-state performance for initial operating conditions

Figures 2–5 present the distributions of some

variables of the SOFC along the cell length direction under the initial operating conditions. In these figures, the spatial coordinates have been made dimensionless for better illustration. Fig. 2 gives the molar fraction distributions of all the gas species in the anode channels. It can be seen that after the fuel stream is fed into the anode channels, the molar fractions of CH_4 and H_2O decrease rapidly, while that of H_2 increases rapidly. This indicates that the steam reforming reaction is much faster at the inlet of the anode channels because of the high content of CH_4 there. The CH_4 is consumed gradually and is almost exhausted when z^* is larger than 0.6. After reaching their respective extrema, the molar fractions of H_2O and H_2 start to increase and decrease, respectively. This indicates that, because of the consumption of CH_4 , the reforming reaction grows weak, while the hydrogen oxidation reaction, which consumes H_2 and produces H_2O , becomes dominant. At the anode outlet, the composition of the gas stream is 67.73% in H_2O , 12.39% in H_2 , 3.49% in CO , and 16.39% in CO_2 .

Figure 3 gives the temperature distributions of the anode and cathode gas phase, and the SOLID. It can be seen that these temperatures all decrease at the inlet of the fuel cell because of the cooling effect associated with the endothermic steam reforming reaction. Particularly, the anode gas temperature sharply decreases by more than 65 K in relation to its inlet value within a distance of several millimeters. As the steam reforming reaction grows weak and the exothermic hydrogen oxidation becomes dominant, these temperatures start to increase along the gas flow direction, with their maximum temperatures occurring at the cell outlet. The maximum and minimum SOLID

Table 4 Parameters used in simulation

	Parameter	Value
dimensions of the cell [5, 10]	cell length/m	0.1
	cell width/m	0.1
	anode thickness/m	500×10^{-6}
	cathode thickness/m	50×10^{-6}
	electrolyte thickness/m	20×10^{-6}
	interconnect thickness/m	500×10^{-6}
	fuel channel height/m	1.0×10^{-3}
material properties of the cell [10]	air channel height/m	1.0×10^{-3}
	anode electrical conductivity/ $\Omega^{-1} \cdot \text{m}^{-1}$	8.0×10^4
	cathode electrical conductivity/ $\Omega^{-1} \cdot \text{m}^{-1}$	8.0×10^3
	electrolyte ionic conductivity/ $\Omega^{-1} \cdot \text{m}^{-1}$	$3.34 \times 10^4 \exp(-10300/T)$
	PEN density/ $\text{kg} \cdot \text{m}^{-3}$	5900
	PEN heat capacity/ $\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$	500
	PEN thermal conductivity/ $\text{J} \cdot \text{s}^{-1} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	2
	interconnect density/ $\text{kg} \cdot \text{m}^{-3}$	8000
	interconnect heat capacity/ $\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$	500
	interconnect thermal conductivity/ $\text{J} \cdot \text{s}^{-1} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$	25
activation and concentration overpotentials	activation energy of anode/ $\text{J} \cdot \text{mol}^{-1}$	140000
	activation energy of cathode/ $\text{J} \cdot \text{mol}^{-1}$	137000
	pre-exponential coefficient for anode in Eq. (31)/ $\text{A} \cdot \text{m}^{-2}$	8.0×10^{10}
	pre-exponential coefficient for cathode in Eq. (32)/ $\text{A} \cdot \text{m}^{-2}$	1.5×10^{10}
	limiting current density/ $\text{A} \cdot \text{m}^{-2}$	12000
initial operating conditions	average current density/ $\text{A} \cdot \text{m}^{-2}$	5000
	fuel utilization	0.8
	air ratio	7.5
	pressure/Pa	1.0×10^5
	inlet fuel temperature/K	1023
	inlet air temperature/K	1023
	inlet fuel composition	$\text{CH}_4 : 0.33, \text{H}_2\text{O} : 0.67$
	inlet air composition	$\text{O}_2 : 0.21, \text{N}_2 : 0.79$
numerical solution	node number	100

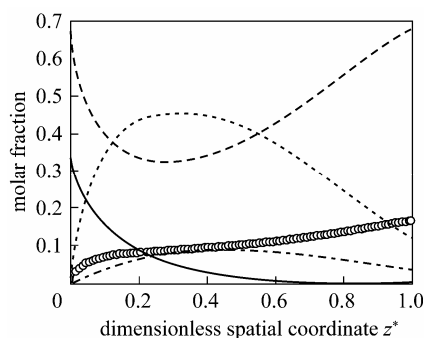


Figure 2 Steady-state molar fraction distributions of the anode gas species for the initial operating conditions in Table 4

— CH_4 ; ---- H_2O ; H_2 ; -.-.- CO ; ○ CO_2

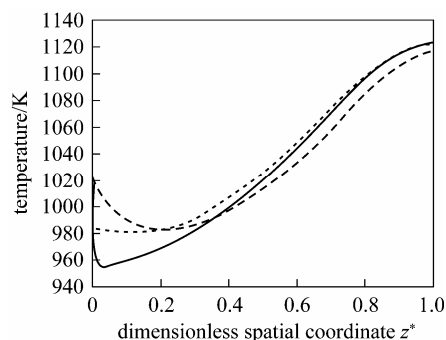


Figure 3 Steady-state temperature distributions of the anode and cathode gas phase, and the SOLID for the initial operating conditions in Table 4

— anode gas phase; ---- cathode gas phase; SOLID

temperature is 1122 and 980 K, respectively, leading to a maximum temperature difference of approximately 142 K.

As the thin film of the PEN is brittle and is apt to be damaged by excessive thermally induced stresses

within it, attention should be paid to the temperature gradients of the PEN along the cell. The present model can calculate the temperature gradient distribution of the SOLID (see Fig. 4), which can reflect that of the PEN to a certain extent. It can be seen from Fig. 4 that

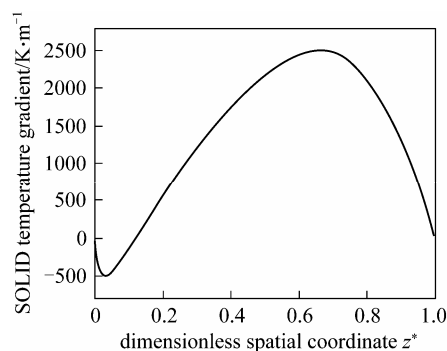


Figure 4 Steady-state temperature gradient distribution of the SOLID for the initial operating conditions in Table 4

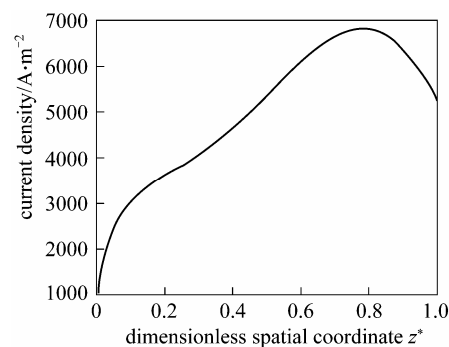


Figure 5 Steady-state current density distribution for the initial operating conditions in Table 4

there exist two extrema of the SOLID temperature gradient. The smaller one, which is near the cell inlet, results from the endothermic reforming reaction, whereas the larger one is because of the heat accumulation along the cell length direction. The trend of this curve is reasonable.

Figure 5 illustrates the current density distribution along the cell. The current density depends on the H_2 molar fraction as well as on the cell temperature. At the cell inlet, the current density is quite low because of the low H_2 content and cell temperature there. With the H_2 molar fraction and the cell temperature increasing along the cell, the current density gradually increases and reaches its maximum at approximately $z^* = 0.8$. Note that the current density maximum lies behind the H_2 molar fraction maximum because of the cell temperature increase (see also Figs. 2 and 3). Then, the current density starts to decrease because of the low H_2 content.

From the analysis on Figs. 2–5, it can be found that introducing the direct internal reforming has sig-

nificant effects on the distributions of these variables. These profiles are in agreement with those reported by Aguiar *et al.* [10] and Nikooyeh *et al.* [5] using different SOFC models. Under this steady state, the SOFC has a voltage of 0.658V and an electrical efficiency of 50.7% (low heat value, LHV).

5.2 Transient behavior analysis

In this sub-section, the dynamic response of the SOFC to disturbances in several operating parameters, including the load current, and the inlet fuel and air flow rates, is analyzed with the above steady state as the initial state. For each operating parameter, both its step-decrease and step-increase are considered.

5.2.1 Responses to step-changes in load

The following load disturbances are imposed on the SOFC: at $t = 100$ s, the average current density instantaneously changes from 5000 to 4000 and 6000 $A \cdot m^{-2}$. Figs. 6–9 illustrate the corresponding dynamic

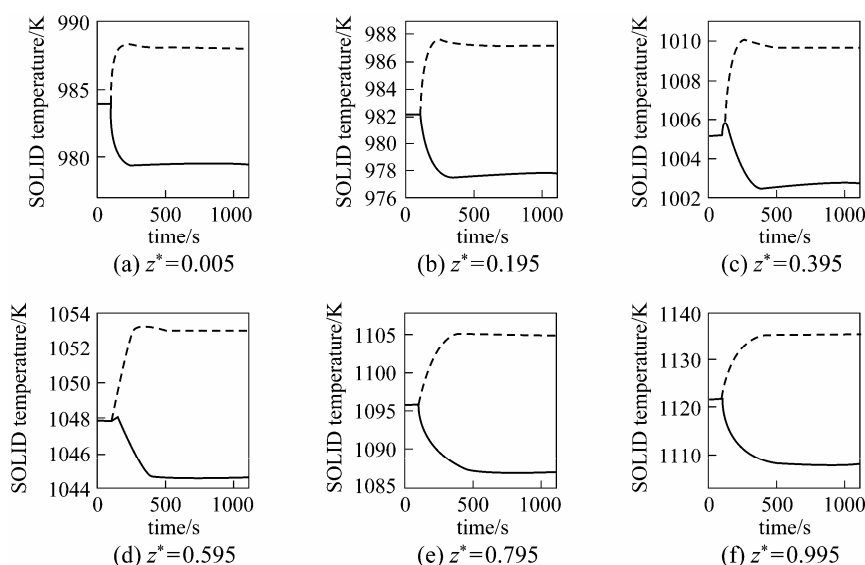


Figure 6 Dynamic responses of the SOLID temperature for load current step-changes from 5000 (initial steady-state value) to 4000 and 6000 $A \cdot m^{-2}$. — step-change to 4000 $A \cdot m^{-2}$; ---- step-change to 6000 $A \cdot m^{-2}$

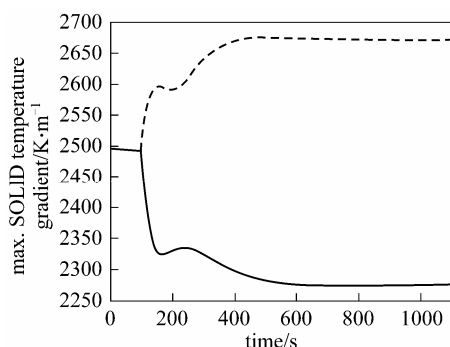


Figure 7 Dynamic responses of the maximum SOLID temperature gradient for load current step-changes from 5000 (initial steady-state value) to 4000 and 6000 $\text{A}\cdot\text{m}^{-2}$ — step-change to 4000 $\text{A}\cdot\text{m}^{-2}$; ---- step-change to 6000 $\text{A}\cdot\text{m}^{-2}$

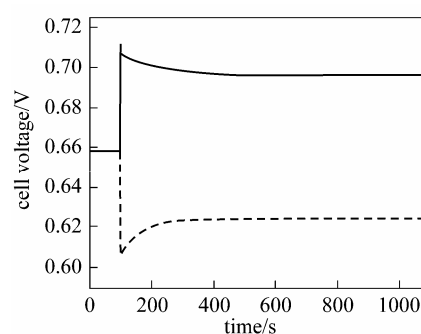


Figure 9 Dynamic responses of the cell voltage for load current step-changes from 5000 (initial steady-state value) to 4000 and 6000 $\text{A}\cdot\text{m}^{-2}$ — step-change to 4000 $\text{A}\cdot\text{m}^{-2}$; ---- step-change to 6000 $\text{A}\cdot\text{m}^{-2}$

responses of the SOLID temperature, the maximum SOLID temperature gradient, the local current density, and the cell voltage, respectively. For the convenience of showing the transient behavior of spatially distributed variables, six positions in the z^* -axis are chosen.

From Figs. 6 and 7, it can be seen that the SOLID temperature of each position and the maximum SOLID temperature gradient both decrease for the step-decrease in the average current density and both increase for its step-increase. The transient process of the SOLID temperature lasts approximately 400–600 s.

It can be seen from Fig. 8 that when the step-decrease/step-increase in the average current density occurs, the current density of each position has a pronounced instantaneous decrease/increase, followed by slight variations because of the SOLID temperature dynamics. At last, the current density of each position stabilizes at a lower/higher level than its

initial value. In addition, it can also be found that the transient behavior of the local current density varies with the position.

It can be seen from Fig. 9 that when the average current density step-decrease occurs, the cell voltage first increases instantaneously, then gradually goes down, and finally, stabilizes at a new steady-state value higher than the initial voltage. The dynamic response of the cell voltage is characterized by an overshoot. This phenomenon can be explained as: immediately after the average current density decreases, the cell temperature is still high, while various overpotentials become lower at that point. The lower amount of waste heat produced at the lower average current density (*i.e.*, 4000 $\text{A}\cdot\text{m}^{-2}$) causes the cell temperature to go down, which results in the gradual decrease in the cell voltage because of the cell overpotential increase. For the average current density step-increase, the cell

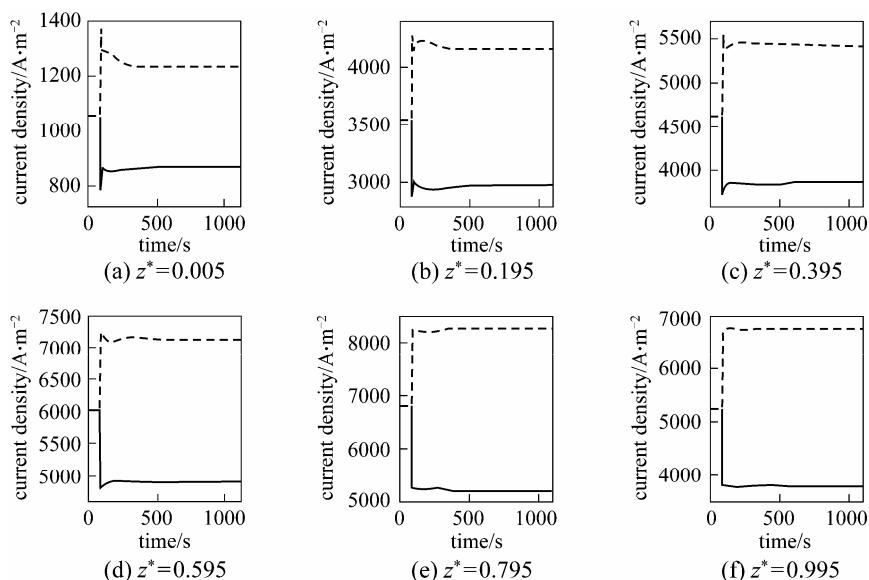


Figure 8 Dynamic responses of the local current density for load current step-changes from 5000 (initial steady-state value) to 4000 and 6000 $\text{A}\cdot\text{m}^{-2}$ — step-change to 4000 $\text{A}\cdot\text{m}^{-2}$; ---- step-change to 6000 $\text{A}\cdot\text{m}^{-2}$

voltage response shows the opposite trend.

5.2.2 Responses to step-changes in inlet fuel flow rate

The following disturbances in the inlet fuel flow rate are imposed on the SOFC: at $t = 100$ s, the fuel utilization instantaneously changes from 0.8 to 0.7 and 0.9.

Figure 10 presents the corresponding dynamic response of the SOLID temperature. It can be seen that after the fuel utilization step-decrease, the SOLID temperature of each position decreases. This is because the amounts of heat absorbed by the steam reforming reaction and transferred by convection both increase because of the inlet fuel flow rate increase. In

addition, it is worth noting that the SOLID temperature at the cell outlet has a slight increase before it decreases [Fig. 10 (f)]. The transient behavior is not owned by the SOLID temperature responses of other positions. From the current density dynamic response, shown in Fig. 11, it can be found that this SOLID temperature increase is related to the local current density increase there.

Figure 11 presents the corresponding dynamic response of the local current density. After the fuel utilization step-decrease, the current density of each position has a rapid change because of changes in the H_2 and H_2O molar fractions, followed by slow variations

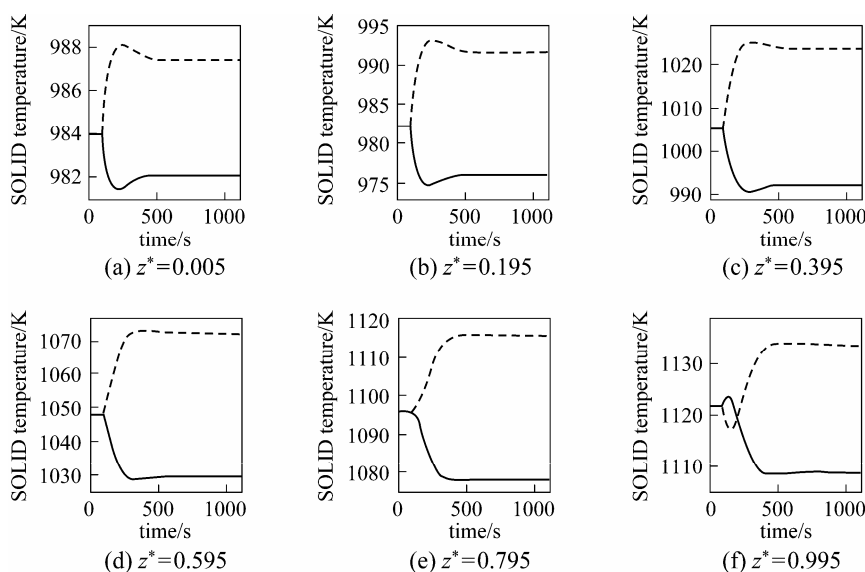


Figure 10 Dynamic responses of the SOLID temperature for fuel utilization step-changes from 0.8 (initial steady-state value) to 0.7 and 0.9

— step-change to 0.7; ---- step-change to 0.9

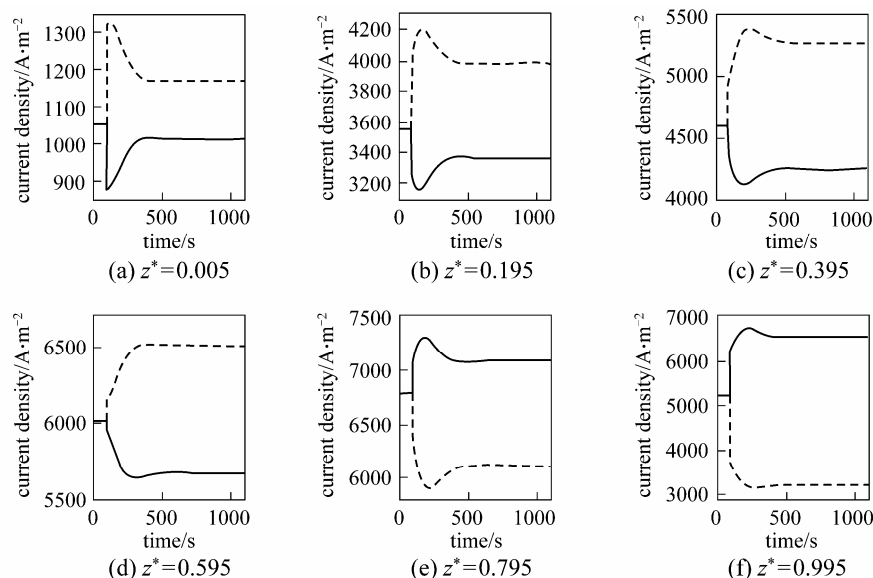


Figure 11 Dynamic responses of the local current density for fuel utilization step-changes from 0.8 (initial steady-state value) to 0.7 and 0.9

— step-change to 0.7; ---- step-change to 0.9

resulting from the SOLID temperature dynamics. Finally, the current densities of some positions increase, while those of some positions decrease. This indicates that the current density distribution might change because of the fuel utilization change. This conclusion can be corroborated by Fig. 12, which illustrates the steady-state current density distributions for different fuel utilizations.

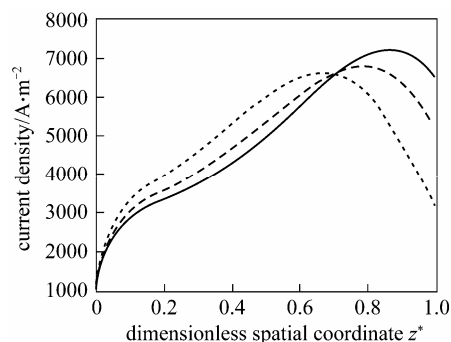


Figure 12 Steady-state current density distributions for different fuel utilizations
(The other operating parameters are their initial values in Table 4)
fuel utilization: — 0.7; ---- 0.8; 0.9

Figure 13 presents the corresponding dynamic response of the cell voltage. It can be seen that after the fuel utilization step-decrease, the cell voltage first increases instantaneously, and then, gradually decreases to a new steady-state value lower than its initial value. An overshoot can also be observed from the response curve of the cell voltage. The instantaneous voltage increase is caused by the H_2 molar fraction increase arising from the fuel flow rate increase and the subsequent voltage decrease results from the cell temperature decrease.

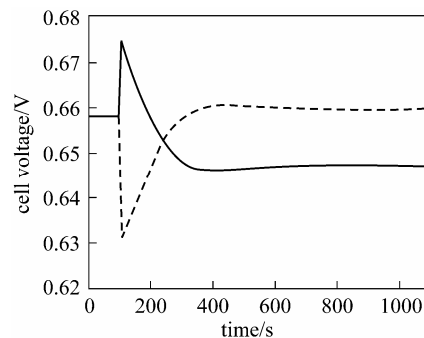


Figure 13 Dynamic responses of the cell voltage for fuel utilization step-changes from 0.8 (initial steady-state value) to 0.7 and 0.9

— step-change to 0.7; ---- step-change to 0.9

In addition, from Figs. 10, 11, and 13, it can also be found that the responses of the SOLID temperature, local current density, and cell voltage to the fuel utilization step-increase show the opposite trends to those of the fuel utilization step-decrease.

5.2.3 Responses to step-changes in inlet air flow rate

The following disturbances in the inlet air flow rate are imposed on the SOFC: at $t=100$ s, the air ratio instantaneously changes from 7.5 to 5.5 and 9.5.

Figures 14 and 15 present the corresponding dynamic responses of the SOLID temperature and the local current density, respectively. It can be seen that after the air ratio changes, the SOLID temperatures and local current densities of some positions decrease, while those of some positions increase. These figures indicate that the inlet air flow rate change leads to the changes in the distributions of the SOLID temperature and the current density. In addition, it can be found from Fig. 15 that the current density dynamic process

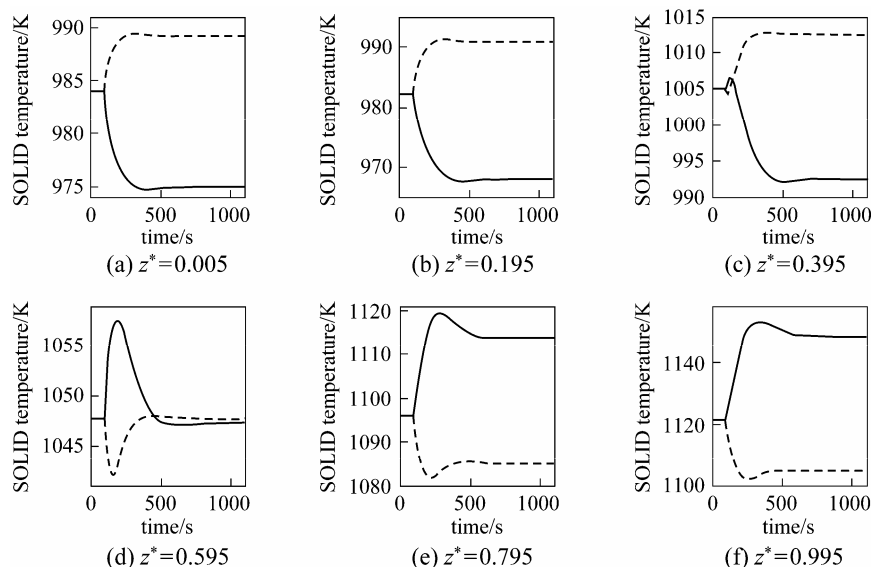


Figure 14 Dynamic responses of the SOLID temperature for air ratio step-changes from 7.5 (initial steady-state value) to 5.5 and 9.5

— step-change to 5.5; ---- step-change to 9.5

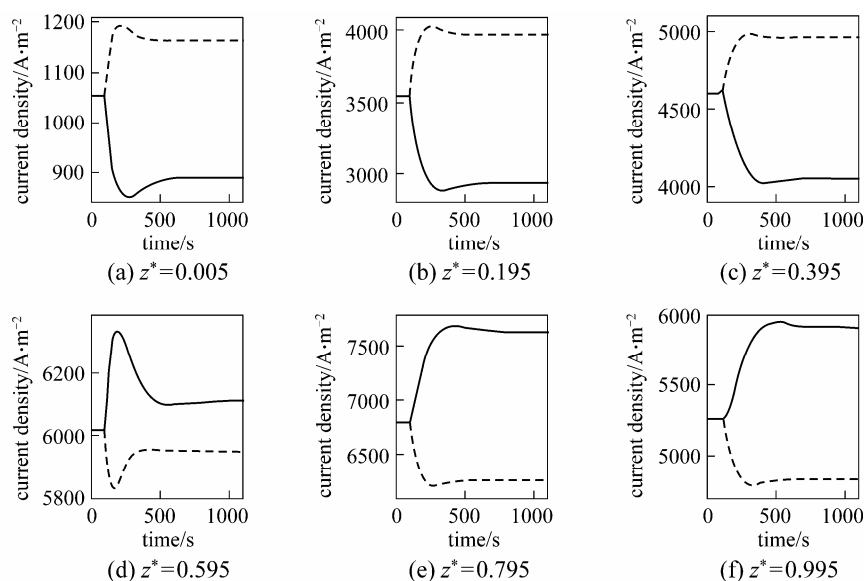


Figure 15 Dynamic responses of the local current density for air ratio step-changes from 7.5 (initial steady-state value) to 5.5 and 9.5

— step-change to 5.5; ---- step-change to 9.5

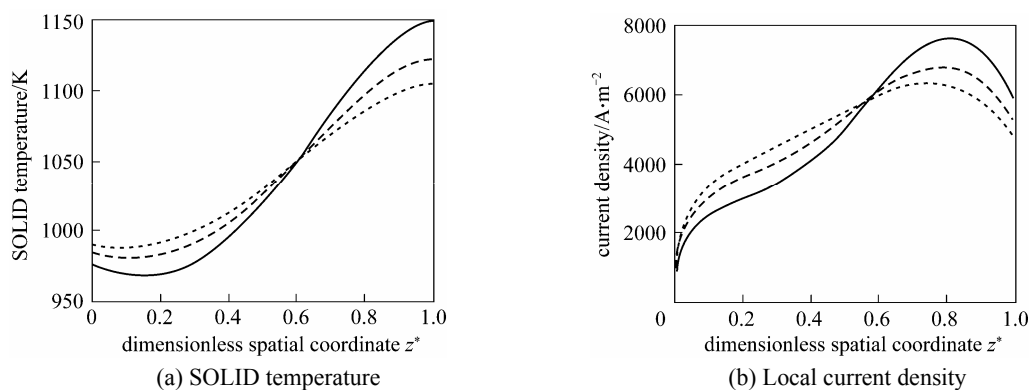


Figure 16 Steady-state distributions of the SOLID temperature and the local current density for different air ratios (The other operating parameters are their initial values in Table 4)

air ratio: — 5.5; ---- 7.5; 9.5

is mainly caused by the SOLID temperature dynamics, while the effect of the O_2 molar fraction change, which results from the inlet air flow rate change, on the current density is hardly noticeable.

To show the impact of the air ratio more clearly, Fig. 16 presents the steady-state distributions of the SOLID temperature and the local current density for different air ratios. It can be seen that the air ratio decrease can lead to steeper SOLID temperature profiles and to more uneven current density distributions, and its increase can flat the SOLID temperature and the current density distributions. Table 5 lists the corresponding maximum temperature, maximum temperature difference, and maximum temperature gradient of the SOLID for different air ratios. It can be seen that, with the air ratio increase, these variables all go down. This is the reason why the inlet air flow rate is often manipulated to control the cell temperature.

Figure 17 presents the corresponding dynamic

response of the cell voltage for the air ratio disturbances. It can be found that when the air ratio step-decrease/

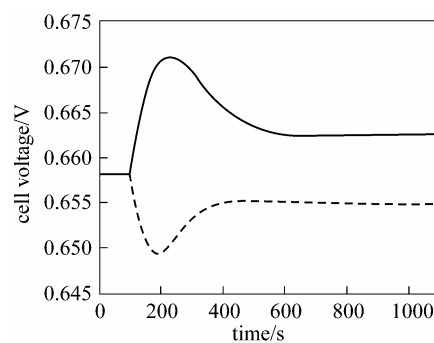


Figure 17 Dynamic responses of the cell voltage for air ratio step-changes from 7.5 (initial steady-state value) to 5.5 and 9.5

— step-change to 5.5; ---- step-change to 9.5

Table 5 Maximum temperature, temperature difference and temperature gradient of the SOLID for different air ratios

Air ratio	Max. SOLID temperature/K	Max. SOLID temperature difference/K	Max. SOLID temperature gradient/K·m ⁻¹
5.5	1149.2	182.0	3440.8
7.5	1121.8	141.5	2493.8
9.5	1105.0	117.4	1943.6

Note: The other operating parameters are their initial values given in Table 4.

step-increase is introduced, the cell voltage first has a tiny step-decrease/step-increase, and then, undergoes a slow transient process characterized by an overshoot/undershoot. The tiny voltage step-decrease/step-increase is caused by the O₂ molar fraction decrease/increase arising from the inlet air flow rate decrease/increase and the subsequent slow transient process results from the SOLID temperature dynamics.

6 CONCLUSIONS

A one-dimensional dynamic planar DIR-SOFC model has been developed based on mass and energy balances, and electrochemical principles. The model is able to predict some SOFC variables, including the cell temperature, the gas molar fractions, the cell voltage, and the current density along the cell length as well as their variation with time. The effectiveness of the present model has been verified by using the IEA benchmark test. Through model-based simulations, the steady-state performance of a co-flow planar DIR-SOFC under specified initial operating conditions and its dynamic response to the step-changes in several operating parameters including the load current, and the inlet fuel and air flow rates have been investigated. From the analysis of the simulation results, the following main conclusions can be drawn:

(1) The direct internal reforming process has significant effect on the distributions of the anode gas composition, cell temperature, SOLID temperature gradient, and current density along the cell length direction.

(2) Because of the spatially distributed property of the cell temperature and the current density, their transient behavior varies with the position.

(3) The rapid dynamics of the current density and the cell voltage are mainly influenced by the gas composition, particularly the H₂ molar fraction in anode gas channels, whereas their slow dynamics are both dominated by the SOLID temperature.

(4) As the load current increases, the SOLID temperature and the maximum SOLID temperature gradient both increase. Thereby, the cell breakdown is apt to occur because of excessive thermally induced stresses.

(5) Changing the inlet fuel flow rate might lead to the change in the anode gas composition and the consequent changes in the current density distribution and the cell voltage.

(6) The inlet air flow rate has a great impact on

the cell temperature distribution along the cell. Its decrease can result in a steeper SOLID temperature distribution, whereas its increase can make the SOLID temperature distribution flat, leading to decreases in the maximum temperature, maximum temperature gradient, and maximum temperature difference of the SOLID. Therefore, the inlet air flow rate is a suitable manipulated variable to control the cell temperature.

NOMENCLATURE

A	area, m ²
$a_{i,k}$	stoichiometric vector of species i in stream k in reactions (i)–(iv)
a_k	total stoichiometric vector of stream k in reactions (i)–(iv)
C	gas molar concentration, mol·m ⁻³
$c_{p,i}$	molar specific heat capacity of gas species i , J·mol ⁻¹ ·K ⁻¹
$c_{p,s}$	mass specific heat capacity of the SOLID, J·kg ⁻¹ ·K ⁻¹
E_A	activation energy, J·mol ⁻¹
F	Faraday constant, C·mol ⁻¹
ΔH	reaction enthalpy change at the temperature of 298.15 K, J·mol ⁻¹
h	gaseous molar specific enthalpy, J·mol ⁻¹
J	average current density, A·m ⁻²
j	local current density, A·m ⁻²
K_{sh}	equilibrium constant of WGS reaction
k_r	steam reforming reaction constant, mol·s ⁻¹ ·m ⁻² ·Pa ⁻¹
$k_{s,a}, k_{s,c}$	convective heat transfer coefficients between gas streams and the SOLID, J·s ⁻¹ ·m ⁻² ·K ⁻¹
k_{sh}	WGS reaction constant
L	cell length, m
$l_{s,a}, l_{s,c}$	total sectional perimeter of anode, cathode gas channels, m
N	molar flow rate, mol·s ⁻¹
n	node number
n_e	number of electrons transferred per electrochemical reaction
P	pressure, Pa
R	universal gas constant
R_{ohm}	cell internal resistance, Ω·m ²
r_j	reaction rate of reaction j , mol·s ⁻¹ ·m ⁻²
S_h	heat source term, J·s ⁻¹ ·m ⁻³
S_m	mass source term, mol·s ⁻¹ ·m ⁻³
T	temperature, K
U	cell operating voltage, V
U_{OCV}	open circuit voltage, V
U_0	open circuit voltage at the standard pressure, V
W	cell width, m
$x_{i,k}$	molar fraction of gas species i in stream k
z	spatial coordinate, m
β_a, β_c	pre-exponential coefficient for anode and cathode in Eqs. (31) and (32), A·m ⁻²
ζ_k	number of gas species in stream k
η	overpotential, V
λ	thermal conductivity, J·s ⁻¹ ·m ⁻¹ ·K ⁻¹
ρ	density, kg·m ⁻³
$\sigma_a, \sigma_c, \sigma_{el}$	electrical conductivity of anode, cathode and electrolyte, Ω ⁻¹ ·m ⁻¹
$\tau_a, \tau_c, \tau_{el}$	thickness of anode, cathode and electrolyte, m
Superscripts	
ref	reference condition (298.15 K, 1.0×10 ⁵ Pa)
0	inlet gas conditions

* dimensionless

Subscripts

a	anode
act	activation
c	cathode
con	concentration
<i>i</i>	gas species <i>i</i>
int	interconnect
<i>j</i>	reaction <i>j</i>
<i>k</i>	gas stream <i>k</i>
ohm	ohmic
PEN	PEN structure
r	steam reforming reaction
s	SOLID
sh	WGS reaction

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