

# The modeling of a standalone solid-oxide fuel cell auxiliary power unit

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## Abstract

In this research, a Simulink model of a standalone vehicular solid-oxide fuel cell (SOFC) auxiliary power unit (APU) is developed. The SOFC APU model consists of three major components: a controller model; a power electronics system model; and an SOFC plant model, including an SOFC stack module, two heat exchanger modules, and a combustor module. This paper discusses the development of the nonlinear dynamic models for the SOFC stacks, the heat exchangers and the combustors. When coupling with a controller model and a power electronic circuit model, the developed SOFC plant model is able to model the thermal dynamics and the electrochemical dynamics inside the SOFC APU components, as well as the transient responses to the electric loading changes. It has been shown that having such a model for the SOFC APU will help design engineers to adjust design parameters to optimize the performance. The modeling results of the SOFC APU heat-up stage and the output voltage response to a sudden load change are presented in this paper. The fuel flow regulation based on fuel utilization is also briefly discussed.

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## 1. Introduction

The solid-oxide fuel cell (SOFC) is a type of fuel cell in which the electrolyte is a solid, nonporous metal oxide. The SOFC operates at very high temperatures (600–1000 °C). In the cells, oxygen ions are transferred through a solid-oxide electrolyte material to react with hydrogen on the anode side. Their off-gases are often used to fire a secondary gas turbine to improve electrical efficiency.

The SOFC auxiliary power unit (APU) draws the interest of many researchers because of its high efficiency, low emission, modular structure, and high generation capability. Many SOFC applications are stationary. Recently, the development of an SOFC APU for vehicular usage on long-haul trucks is gaining more and more attention. In this paper, we modeled and simulated a completely standalone SOFC unit fueled by hydrocarbon fuel for control applications.

The technical challenges of designing an SOFC APU controller are

- Thermal management.

- Fuel management.
- Transient and load following characteristics.

Thermal management is critical in maintaining the normal operation of an SOFC system. SOFCs operate at temperatures ranging from 600 to 1000 °C. A standalone SOFC unit should be able to run with fuel and air supplied at their normal storage temperature. The high-temperature working condition requires that the inflow gases need to be heated to their working temperature prior to being fed to the SOFC stacks. As a standalone unit, the SOFC system should be able to heat the inflow gases using the energy generated by combustion of a portion of the inflow gases and/or the exhaust gases. Appropriate amounts of fuel and air heated to their working temperature should be guaranteed without any extra facilities, other than the SOFC unit itself.

Fuel management allows the SOFC to run at a higher efficiency, while the voltage is maintained within the desired range. The transient and load following characteristics of an SOFC stack determine the design of the power electronic circuits.

One of the models discussed in this paper is the electrochemical dynamic model. The electrochemical reaction happens in the SOFC stack. The electrical output of the SOFC can be influenced by power load, fuel and oxidant gas flow rate, temperature, and partial pressure of the reacting gases. The electrochemical

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**Nomenclature**

$A$	area ( $\text{m}^2$ )
$c_i$	specific heat ( $\text{kJ kg}^{-1} \text{K}^{-1}$ )
$C$	discharge coefficient
$C_i$	thermal capacity ( $\text{J K}^{-1}$ )
$E^0$	standard reversible cell potential (V)
$F$	Faraday's constant ( $96485.3415 \text{ C mol}^{-1}$ )
$G$	Gibb's free energy (J)
$\Delta G$	change of Gibb's free energy ( $\text{J s}^{-1}$ )
$H$	enthalpy ( $\text{J mol}^{-1}$ )
$\Delta H$	total enthalpy change caused by chemical reactions ( $\text{J s}^{-1}$ )
$I$	current (A)
$K$	specific heat ratio of the discharged gas
$K_p$	equilibrium constant of the reaction
$m_i$	mass of the flow or one SOFC cell (kg)
$M$	gas molecular weight ( $\text{g mol}^{-1}$ )
$n$	number of moles; or, number of electrons generated in the cell reactions
$n_i$	molar flow rate of species $i$ ( $\text{mol s}^{-1}$ )
$n_i^r$	total rate of production of species $i$ ( $\text{mol s}^{-1}$ )
$n_{\text{stack}}$	number of cells in a stack
$N_0$	number of cells in stack
$p_i$	partial pressure of each component (species $i$ ) (Pa)
$P$	absolute pressure (Pa)
$P_d$	downstream ambient (Pa)
$P_e$	power consumed by the electrical loads ( $\text{J s}^{-1}$ )
$P_s$	absolute source pressure (Pa)
$q$	heat flow ( $\text{J s}^{-1}$ )
$Q$	heat flow rate generated by chemical reactions ( $\text{J s}^{-1}$ ); or, electric charge (C)
$r$	ohmic resistance ( $\Omega$ )
$R$	gas constant ( $8.31451 \text{ kJ kmol}^{-1} \text{K}^{-1}$ )
$R_i$	thermal resistances ( $\text{K s J}^{-1}$ )
$S$	entropy ( $\text{J K}^{-1}$ )
$T$	temperature (K)
$V$	compartment volume ( $\text{m}^3$ )
$V_{\text{anode}}$	over-potential caused by diffusion in the cell anode (V)
$V_{B,V}$	Butler–Volmer over-potential (V)
$V_{\text{cathode}}$	over-potentials caused by diffusion in the cell cathode (V)
$V_i$	volume of the flow ( $\text{m}^3$ )
$V_{\text{Nernst}}$	open-circuit Nernst potential (V)
$V_r$	voltage drop caused by the material resistances (V)
$w_i$	mass flow rate ( $\text{kg s}^{-1}$ )
$W$	electric work ( $\text{J s}^{-1}$ )
$y_i^{\text{in}}$	inlet flow molar fraction of species $i$
<i>Greek letters</i>	
$\alpha_i$	stoichiometric coefficients of species $i$
$\varepsilon$	heat transfer rate
$\rho_i$	density of the flow ( $\text{kg m}^{-3}$ )

dynamic model addresses all these factors, which influence the electrical output.

There is a great deal of literature addressing individual aspects of this modeling problem, such as the thermo-fluid modeling [1], flow modeling [2], and the modeling of dynamic responses of fuel cells [3–9]. However, very few researchers have developed a complete system model for a standalone SOFC stack, including dynamic models for auxiliary equipment such as the combustor, heat exchangers, the reformer and power electronic circuits. A complete system model allows researchers to test different control schemes, adjust design parameters of each component, observe dynamic responses of the APU, and tackle the three technical challenges in controller design mentioned above. Therefore, it is critical to build such a model for the purpose of the SOFC APU control applications.

This paper is the first of a series of articles on this topic, in which we present a Simulink model comprising four modules: the SOFC stack module, the combustor module, the heat exchanger module, and the controller logic layer, as shown in Fig. 1. It is assumed in this paper that the SOFC stack is fueled by hydrogen, so that no reformer is included in the model. The focus of the paper is to derive mathematical models for each individual component and integrate these individual models into a complete SOFC model using Simulink. A control logic system as a separate layer in the Simulink model was developed to monitor the normal working condition of the SOFC stacks, regulate the gas flows according to power consumption requirement, and control the combustor and the heat exchangers. The simulation of the power electronic system load following characteristics will be presented in follow-up publications, in which different controller design schemes and the module of power electronic circuits will be presented.

## 2. Calculations and results

In Sections 2.1–2.3, we present the SOFC stack, the combustor and the heat exchanger modules. Simulation results are reported in Section 2.4.

### 2.1. The SOFC stack module

Two dynamic responses are considered in modeling the SOFC stack: the thermal dynamics and the electrochemical dynamics.

#### 2.1.1. Modeling thermal dynamics inside an SOFC stack

To calculate the SOFC stack temperature, a detailed and accurate computational fluid dynamics (CFD) model, as shown in Fig. 2(a), can be used to simulate every cell in great detail and to obtain the temperature gradient of each cell [1]. However, this method is quite involved and takes a significant amount of computational time to complete; thus, it is not applicable for dynamic modeling of an SOFC system and real-time controller design. For control applications, it is not necessary to have such great accuracy because the feedback will correct a considerable amount of error in the model. Therefore, it makes sense to com-

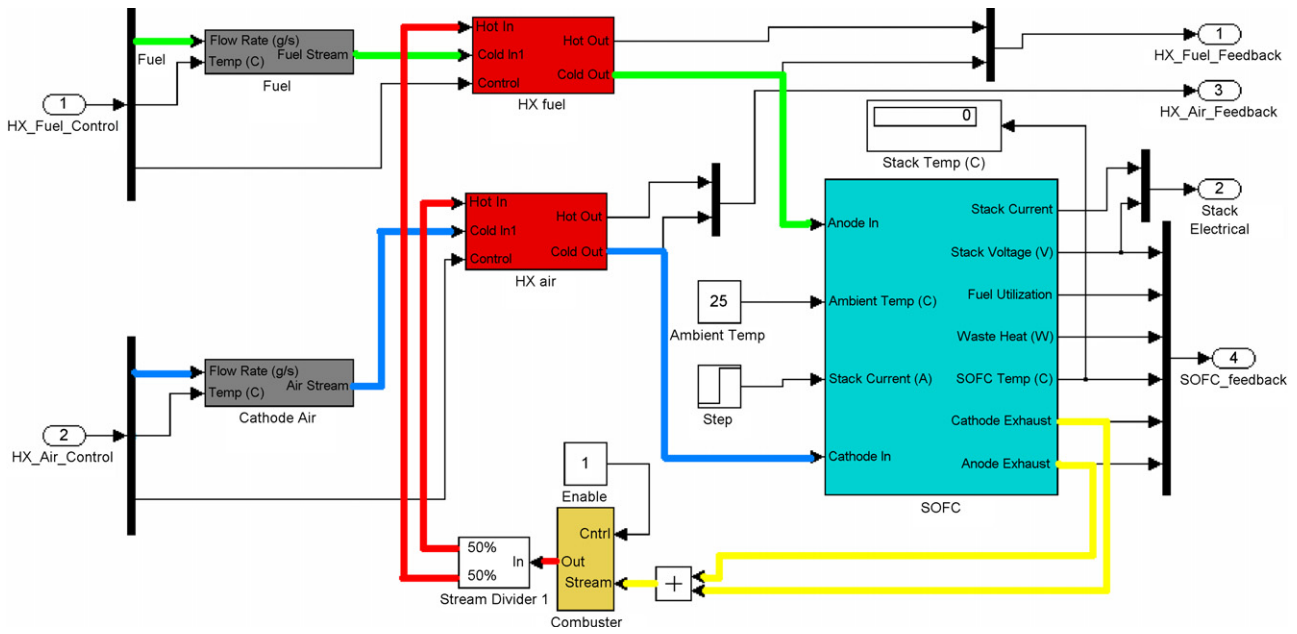


Fig. 1. The block diagram of a solid-oxide fuel cell auxiliary power unit.

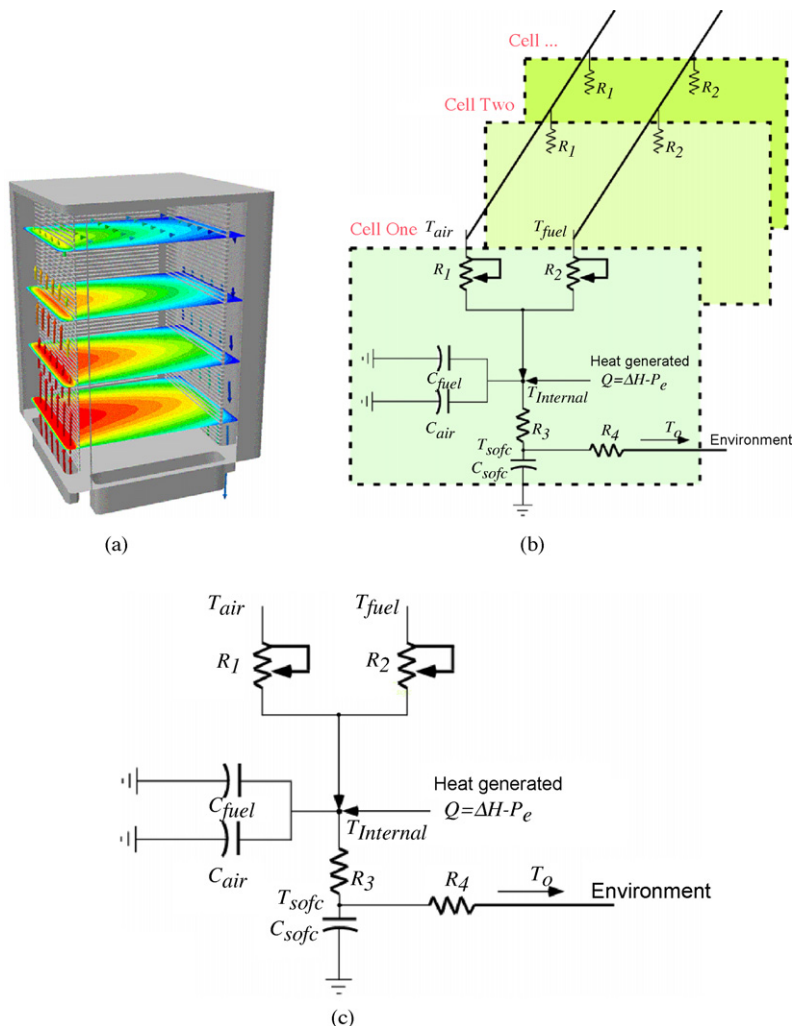


Fig. 2. (a) Fuel cell stacks, (b) a distributed thermal model, and (c) a lumped thermal model.

bine the spatially varying temperatures into single temperatures  $T_{\text{air}}$ ,  $T_{\text{fuel}}$  and  $T_{\text{sofc}}$  for the inflow air, fuel, and the SOFC stack temperatures, respectively. Another temperature that was used in the SOFC modeling is  $T_{\text{Internal}}$ , which represents the temperature inside a cell, where chemical reactions happen. It is noted that temperature sensors cannot measure  $T_{\text{Internal}}$  directly.  $T_{\text{sofc}}$  is the sensor-measured SOFC stack temperature signal, which can be sent to the controller. The simplification results in a distributed lumped model, as shown in Fig. 2(b). An aggregated lumped model can be obtained by aggregating the distributed lumped model for each cell, as shown in Fig. 2(c).

The heat flow  $q$  transferred from the air and fuel to the SOFC stack can be represented as

$$q_{\text{air}} = w_{\text{air}}c_{\text{va}}(T_{\text{air}} - T_{\text{Internal}}) = \frac{1}{R_1}(T_{\text{air}} - T_{\text{Internal}}),$$

$$q_{\text{fuel}} = w_{\text{fuel}}c_{\text{vf}}(T_{\text{fuel}} - T_{\text{Internal}}) = \frac{1}{R_2}(T_{\text{fuel}} - T_{\text{Internal}}) \quad (1)$$

where  $R_1 = \frac{1}{w_{\text{air}}c_{\text{va}}}$  and  $R_2 = \frac{1}{w_{\text{fuel}}c_{\text{vf}}}$ .

Also,  $w_{\text{air}}$  and  $w_{\text{fuel}}$  are the air and fuel flow rates, respectively,  $c_{\text{va}}$  and  $c_{\text{vf}}$  the specific heat of air and the fuel, respectively, and  $R_1$  and  $R_2$  are the thermal resistances of the air and fuel flow, respectively. Note that  $R_1$  and  $R_2$  are changing with respect to the air and fuel flow rates. Therefore, they are represented as adjustable resistances in the equivalent electric circuit model.

The heat flow  $Q$  generated by chemical reactions can be calculated by

$$Q = \Delta H - P_e \quad (2)$$

where  $\Delta H$  is the total enthalpy change caused by chemical reactions and  $P_e$  is the power consumed by the electrical loads.

Inside the fuel cell stack, there are air and fuel that have heat capacities of  $C_{\text{air}}$  and  $C_{\text{fuel}}$ , respectively. Some of the heat will dissipate to the ambient and the rest of the heat goes into the SOFC stack. A complete equivalent electric circuit model that describes the whole heat transfer process is shown in Fig. 2(b). Aggregating the distributed models together, a lumped model is obtained, as shown in Fig. 2(c).  $R_3$  is the thermal resistance of the heat flow averaged over the entire stack, and  $R_4$  is the thermal resistance of the fuel cell stack.

The differential equations describing the lumped model are written as

$$(C_{\text{fuel}} + C_{\text{air}}) \frac{dT_{\text{Internal}}}{dt} = \frac{T_{\text{air}} - T_{\text{Internal}}}{R_1} + \frac{T_{\text{fuel}} - T_{\text{Internal}}}{R_2} + \frac{T_{\text{sofc}} - T_{\text{Internal}}}{R_3} + Q,$$

$$C_{\text{sofc}} \frac{dT_{\text{sofc}}}{dt} = \frac{T_{\text{Internal}} - T_{\text{sofc}}}{R_3} + \frac{T_0 - T_{\text{sofc}}}{R_4} \quad (3)$$

in which, we have

$$C_{\text{fuel}} = m_{\text{fuel}}c_{\text{vf}} = V_{\text{fuel}}\rho_{\text{fuel}}c_{\text{vf}},$$

$$C_{\text{air}} = m_{\text{a}}c_{\text{va}} = V_{\text{air}}\rho_{\text{air}}c_{\text{va}}, \quad C_{\text{sofc}} = m_{\text{cell}}n_{\text{stack}}c_{\text{vsofc}}$$

where  $V_{\text{air}}$  and  $V_{\text{fuel}}$  are volumes of the air and fuel inside the SOFC stack, respectively;  $C_{\text{air}}$ ,  $C_{\text{fuel}}$ , and  $C_{\text{sofc}}$  the thermal

capacitances of the air, the fuel, and the SOFC stack, respectively;  $m_{\text{a}}$ ,  $m_{\text{f}}$ , and  $m_{\text{cell}}$  the mass of the air, the fuel, and one SOFC cell, respectively;  $c_{\text{va}}$ ,  $c_{\text{vf}}$ , and  $c_{\text{vsofc}}$  are specific heat of the air, the fuel, and the SOFC stack, respectively;  $n_{\text{stack}}$  the number of cells in a stack;  $\rho_{\text{air}}$  and  $\rho_{\text{fuel}}$  the density of the air and fuel, respectively.

Let  $C_1 = C_{\text{fuel}} + C_{\text{air}}$  and  $C_2 = C_{\text{sofc}}$ . The state space representation of the model is then written as

$$\dot{X} = AX + Bu, \quad y = CX + Du \quad (4)$$

$$\dot{X} = \begin{bmatrix} \dot{T}_{\text{Internal}} \\ \dot{T}_{\text{sofc}} \end{bmatrix}, \quad X = \begin{bmatrix} T_{\text{Internal}} \\ T_{\text{sofc}} \end{bmatrix}, \quad u = \begin{bmatrix} T_{\text{air}} \\ T_{\text{fuel}} \\ T_0 \\ Q \end{bmatrix},$$

$$A = \begin{bmatrix} -\left(\frac{1}{R_1C_1} + \frac{1}{R_2C_1} + \frac{1}{R_3C_1}\right) & \frac{1}{R_3C_1} \\ \frac{1}{R_3C_2} & -\left(\frac{1}{R_3C_2} + \frac{1}{R_4C_2}\right) \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1}{R_1C_1} & \frac{1}{R_2C_1} & 0 & \frac{1}{C_1} \\ 0 & 0 & \frac{1}{R_4C_2} & 0 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

$$D = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

If the SOFC operating temperature is between 650 and 850 °C, one needs to heat the SOFC stack from room temperature to that temperature range before operation. In the heat-up stage, air flow through the cathode is used to heat the SOFC stack, and fuel will not be fed into the SOFC stack until the stack temperature exceeds 650 °C. The air flow rate,  $w_{\text{air}}$ , and temperature,  $T_{\text{air}}$ , are control variables during the heat-up process. According to CFD simulation results, the temperature gradient of a SOFC should not exceed 100 °C at any time to avoid thermal shock. Therefore, the air flow temperature should follow certain rules such as:

- When  $T_{\text{sofc}} < 650$  °C, the SOFC is running at heat-up mode, the following parameters for the model shall be used:

$$R_2 = 10^6 \text{ J s}^{-1} \text{ K}^{-1}, \quad Q = 0 \text{ J s}^{-1},$$

$$T_{\text{air}} - T_{\text{sofc}} < 100 \text{ }^\circ\text{C} \quad (5)$$

- When  $T_{\text{sofc}} \geq 650$  °C, the SOFC is operating at running mode, the following parameters for the model shall be used:

$$R_2 = \frac{1}{w_{\text{f}}c_{\text{vf}}}, \quad Q = \Delta H - P_e,$$

$$T_{\text{air}} - T_{\text{sofc}} < 50 \text{ }^\circ\text{C} \quad (6)$$

A simulation result of the heat-up process (75–750 °C, air flow 20 g s<sup>-1</sup>) is shown in Fig. 3 The temperature differences are controlled to be within 90–100 °C during the heat-up mode.

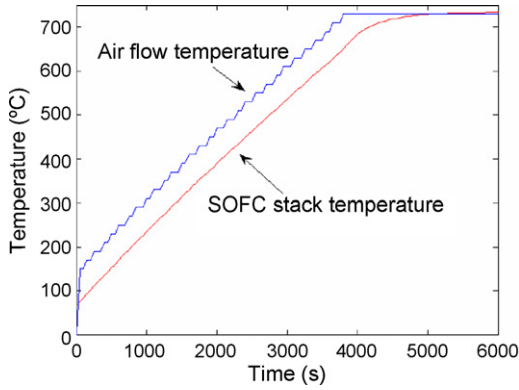
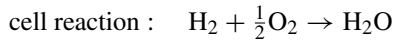
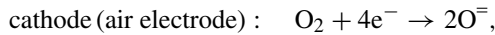


Fig. 3. The temperature dynamics during heat-up.

Because the thermal characteristics of different SOFC stacks may be different, experimental data should be used to assist in tuning the lumped model parameters. Because the temperature difference between  $T_{\text{Internal}}$  and  $T_{\text{sofc}}$  varies no more than  $10^\circ\text{C}$  during the heat-up process, and in steady state  $T_{\text{Internal}}$  and  $T_{\text{sofc}}$  reach the same value, we only plotted the SOFC stack temperature  $T_{\text{sofc}}$ .

### 2.1.2. Modeling electrochemical dynamics inside an SOFC stack

Using hydrogen as fuel, the chemical reactions inside an SOFC stack are:



The electrochemical dynamic inside an SOFC stack can be represented in terms of the change in concentrations of the chemical species in the cell reaction. In our case, the species of interest are  $\text{H}_2$ ,  $\text{O}_2$ , and  $\text{H}_2\text{O}$ . For ideal gases, the concentration changes are equivalent to the partial pressure changes in a fixed volume container. Therefore, in the following sections, starting from the ideal gas equation, we derive a state space model to calculate the partial pressure changes of the chemical species and then use Nernst equation to calculate the voltage changes. An assumption of the derivations is that the cell current can change immediately as long as the fuel and oxygen are not depleted.

**2.1.2.1. Calculate partial pressures of chemical species.** To meet material design and efficiency requirements, the pressure inside the SOFC stack shall not exceed 2–3 atm. Therefore, it is valid to assume that gases inside the SOFC stack behave as ideal gases. For an ideal gas, we have

$$PV = nRT \quad (7)$$

where  $P$  is the absolute pressure,  $T$  the absolute temperature,  $V$  the volume of the gas,  $n$  the number of moles, and  $R$  is the gas constant  $= 8.31451 \text{ kJ kmol}^{-1} \text{ K}^{-1}$ . Then, at any operating temperature  $T$ , the change in partial pressure  $p_i$  of each component

(species  $i$ ) in the reactions can be written as [10]

$$\frac{dPV}{dt} = RT \frac{dn}{dt}, \quad V \frac{dp_i}{dt} = RT \frac{dn_i}{dt},$$

$$\dot{p}_i = \frac{RT}{V} (n_i^{\text{in}} - n_i^{\text{out}} + n_i^r) \quad (8)$$

where  $p_i$  is the partial pressure of species  $i$  (Pa),  $n_i$  is the molar flow rate of species  $i$  ( $\text{mol s}^{-1}$ ),  $n_i^r$  the total rate of production of species  $i$  ( $\text{mol s}^{-1}$ ), and  $V$  is the compartment volume ( $\text{m}^3$ ).

**2.1.2.2. Calculate  $n_i^r$ .** If the SOFC stack current is  $I$  and there are  $N$  cells in a stack,  $n_i^r$  can be calculated as

$$n_i^r = \frac{\alpha_i d \left( \frac{Q}{nF} \right)}{dt} = \alpha_i N \frac{I}{2F} \Rightarrow n_i^r = 2\alpha_i k_r I, \quad k_r = \frac{N}{4F} \quad (9)$$

where  $Q$  is the electric charge transferred during the reaction,  $F$  ( $96485.3415 \text{ C mol}^{-1}$ ) the Faraday's constant, and  $\alpha_i$  is the stoichiometric coefficients of species  $i$ . Note that for the above chemical reactions,  $\alpha = -1$  for  $\text{H}_2$ ;  $\alpha = 1$  for  $\text{H}_2\text{O}$ ; and  $\alpha = -0.5$  for  $\text{O}_2$ .

**2.1.2.3. Calculate  $n_i^{\text{out}}$ .** When gas stored under pressure in a closed vessel is discharged to the atmosphere through a hole or other opening, the gas velocity through that opening may be choked (i.e., has attained a maximum) or non-choked. Choked velocity, which is also referred to as sonic velocity, occurs when the ratio of the absolute source pressure  $P_s$  to the absolute downstream ambient pressure  $P_d$  is equal to or greater than

$$\frac{P_s}{P_d} = \left( \frac{K+1}{2} \right)^{K/(K-1)} \quad (10)$$

where  $K$  is the specific heat ratio of the discharged gas. For many gases,  $K$  ranges from about 1.09 to about 1.41, and thus  $P_s/P_d$  ranges from 1.7 to about 1.9, which means that choked velocity usually occurs when the absolute source vessel pressure is at least 1.7–1.9 times as high as the absolute ambient atmospheric pressure [11–16]. For  $\text{H}_2$  and  $\text{H}_2\text{O}$ , it is reasonable to assume that the orifice is choked because the partial pressures of  $\text{H}_2$  and  $\text{H}_2\text{O}$  are low in atmosphere. For  $\text{O}_2$ , however, depending on the reaction rate and air flow rate, we may or may not treat the orifice as choked.

For a choked orifice, the mass flow rate  $w^{\text{out}}$  can be calculated as

$$w^{\text{out}} = CAP \sqrt{\frac{KM}{RT}} \left( \frac{2}{K+1} \right)^{(K-1)/(2K-2)} \quad (11)$$

where  $w^{\text{out}}$  is the mass flow rate ( $\text{g s}^{-1}$ ),  $C$  is the discharge coefficient (dimensionless, usually about 0.72),  $A$  is the discharge hole area ( $\text{m}^2$ ),  $K$  equals  $c_p/c_v$  of the gas,  $c_p$  is the specific heat at constant pressure,  $c_v$  is the specific heat at constant volume,  $P$  is the absolute source or upstream pressure (Pa),  $M$  is the gas molecular weight ( $\text{g mol}^{-1}$ ),  $R$  is the universal gas law constant, and  $T$  is the gas temperature (K).

Because  $n_i^{\text{out}} = w_i^{\text{out}}/M$ ,

$$n_i^{\text{out}} = \frac{x_i PCA \sqrt{\frac{KM}{RT}} \left(\frac{2}{K+1}\right)^{(K-1)/(2K-2)}}{M} = k_i^{\text{valve}} p_i \quad (12)$$

where  $x_i$  is the molar fraction of species  $i$ , and

$$k_i^{\text{valve}} = \frac{CA \sqrt{\frac{K}{RT}} \left(\frac{2}{K+1}\right)^{(K-1)/(2K-2)}}{\sqrt{M}}$$

The gas molecular weight  $M$  can be calculated by

$$M_{\text{anode}} = x_{\text{H}_2} \left[ \left(1 - \frac{2K_r I}{n_{\text{H}_2}^{\text{in}}}\right) M_{\text{H}_2} + \frac{2K_r I}{n_{\text{H}_2}^{\text{in}}} M_{\text{H}_2\text{O}} \right] + x_{\text{H}_2\text{O}} M_{\text{H}_2\text{O}} \quad (13)$$

For example, if the SOFC operating temperature is 750 °C, the orifice area is 97.96 mm<sup>2</sup>, and the fuel is 97% (molar fraction) H<sub>2</sub> and 3% H<sub>2</sub>O, based on the specific heats of ideal gases in Table 1 [17], the  $K^{\text{valve}}$  is  $1.4298 \times 10^{-7}$  and  $1.4063 \times 10^{-7}$  for H<sub>2</sub> and H<sub>2</sub>O, respectively, under a fuel utilization rate of 0.7.

2.1.2.4. *The electrochemical dynamic model.* Based on Eq. (8), the state space representation of the model is then written as

$$\dot{X} = AX + Bu, \quad Y = CX + Du \quad (14)$$

where

$$X = \begin{bmatrix} p_{\text{H}_2} \\ p_{\text{O}_2}^{\text{cathode}} \\ p_{\text{H}_2\text{O}} \end{bmatrix}, \quad u = \begin{bmatrix} n_{\text{H}_2}^{\text{in}} \\ n_{\text{O}_2}^{\text{in}} \\ n_{\text{H}_2\text{O}}^{\text{in}} \\ I \end{bmatrix},$$

$$A = \begin{bmatrix} \frac{-k_{\text{H}_2}^{\text{valve}} RT}{V_{\text{anode}}} & 0 & 0 \\ 0 & \frac{-k_{\text{O}_2}^{\text{valve}} RT}{V_{\text{cathode}}} & 0 \\ 0 & 0 & \frac{-k_{\text{H}_2\text{O}}^{\text{valve}} RT}{V_{\text{anode}}} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{RT}{V_{\text{anode}}} & 0 & 0 & \frac{-2k_r RT}{V_{\text{anode}}} \\ 0 & \frac{RT}{V_{\text{cathode}}} & 0 & \frac{-k_r RT}{V_{\text{cathode}}} \\ 0 & 0 & \frac{RT}{V_{\text{anode}}} & \frac{2k_r RT}{V_{\text{anode}}} \end{bmatrix},$$

$$C = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

2.1.2.5. *Calculate the Nernst voltage.* Nernst equation allows us to calculate the cell potential of any galvanic cell for any concentration. Assuming ideal gases, for fuel cells that are powered

by H<sub>2</sub>, Nernst equation can be written as

$$V_{\text{Nernst}} = \frac{RT}{4F} \ln \frac{p_{\text{O}_2}^{\text{cathode}}}{p_{\text{O}_2}^{\text{anode}}} \quad (15)$$

Oxygen partial pressure at the anode  $p_{\text{O}_2}^{\text{anode}}$  is calculated by equilibrium constant  $K_p$  of the reaction  $2\text{H}_2 + \text{O}_2 \leftrightarrow 2\text{H}_2\text{O}$ :

$$p_{\text{O}_2}^{\text{anode}} = \left( \frac{p_{\text{H}_2\text{O}}^2}{K_p p_{\text{H}_2}^2} \right) \quad (16)$$

Therefore,

$$V_{\text{Nernst}} = \frac{RT}{4F} \ln \frac{p_{\text{O}_2}^{\text{cathode}} K_p p_{\text{H}_2}^2}{p_{\text{H}_2\text{O}}^2} = \frac{RT}{4F} \ln \frac{p_{\text{O}_2}^{\text{cathode}} p_{\text{H}_2}^2(\text{anode})}{p_{\text{H}_2\text{O}}^2(\text{anode})} + \frac{RT}{4F} \ln K_p \quad (17)$$

For an isothermal reaction, we have

$$E_T^0 = \frac{RT}{4F} \ln K_p \quad (18)$$

Because the operating temperature range is between 650 and 850 °C for the lumped model, we use  $E^0$  value at 750 °C, which is 1023 K. Then, the Nernst equation can be simplified as

$$V_{\text{Nernst}} = N_0 \left( E_{1023}^0 + \frac{RT}{2F} \ln \frac{p_{\text{H}_2} p_{\text{O}_2}^{1/2}}{p_{\text{H}_2\text{O}}} \right) \quad (19)$$

where  $V_{\text{Nernst}}$  is the open-circuit Nernst potential (in V),  $E^0$  the standard reversible cell potential,  $p_{\text{H}_2}$  the partial pressure of H<sub>2</sub> at anode,  $p_{\text{H}_2\text{O}}$  the partial pressure of H<sub>2</sub>O at anode,  $p_{\text{O}_2}$  the partial pressure of O<sub>2</sub> at cathode,  $r$  the ohmic resistance (in Ω),  $F$  the Faraday's constant (Coulomb per kilomole),  $T$  the stack temperature (in K), and  $N_0$  is the number of cells in stack.

2.1.2.6. *Calculate  $E^0$ .*  $K_p$  can be calculated by the Lewis equation:

$$\Delta G_{r,T} = -RT \ln K_p \Rightarrow K_p = e^{-\Delta G_{r,T}/RT},$$

$$E_T^0 = \frac{RT}{4F} \ln K_p = \frac{RT}{4F} \frac{-\Delta G_{r,T}}{RT} = \frac{-\Delta G_{r,T}}{4F} \quad (20)$$

Actually, the change of Gibb's free energy  $\Delta G$  is the negative value of maximum electric work  $W$ , where  $\Delta G = -W = -q\Delta E$ . At standard conditions (298.15 K (25 °C), 1 atm),

$$\Delta_r G^\circ = -nF \Delta E^0 \quad (21)$$

where  $n$  is the number of moles of electrons generated in the cell reactions. From the definitions of Gibb's free energy

$$G \equiv H - TS \Rightarrow \Delta_r G^\circ = \Delta_r H^\circ - T\Delta_r S^\circ \quad (22)$$

where  $H$  is the enthalpy,  $S$  the entropy, and  $T$  is temperature. Therefore,

$$E^0 = \frac{\Delta_r H^\circ - T\Delta_r S^\circ}{nF} \quad (23)$$

Table 1  
Thermodynamic data for the chemical species in the SOFC stack

Chemical species	$c_p$ (kJ kg <sup>-1</sup> K <sup>-1</sup> ) ( $T=750^\circ\text{C}$ )	$c_v$ (kJ kg <sup>-1</sup> K <sup>-1</sup> ) ( $T=750^\circ\text{C}$ )	$\Delta_r H^\circ$ (J mol <sup>-1</sup> ) ( $T=750^\circ\text{C}$ )	$S^\circ$ (J K <sup>-1</sup> mol <sup>-1</sup> ) ( $T=750^\circ\text{C}$ )
H <sub>2</sub>	14.645	10.521	0	166.8831
O <sub>2</sub>	1.043	0.783	0	244.3544
H <sub>2</sub> O	1.8723	1.4108	-247956	233.7132

Relevant thermodynamic data for reactants and products of the chemical reactions have been listed in Table 1 [17]. At 750 °C, for  $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$ , we have  $E^0 = 0.9915\text{ V}$

$$E_{1023}^0 = \frac{-\Delta G_{r,1023}}{4F} = \frac{-2 \times (-191326.3)}{4 \times 96485} = 0.9915\text{ V} \quad (24)$$

Note: The value of  $\Delta_r G_{r,1023}$  is from the thermodynamic properties table [18]. It is multiplied by 2 because there are 2 mol H<sub>2</sub>O in the reaction.

The operating temperature ranges from 650 to 850 °C (923–1123 K). Using 1023 K as a reference temperature [8], the following formula can be used to calculate  $E^0$  at different temperatures:

$$\Delta E_T^0 = \Delta E_{1023}^0 + \frac{\Delta_r S^\circ}{4F}(T - 1023) \quad (25)$$

2.1.2.7. Calculate Nernst voltage using partial pressure. Solving the state space model developed in previous sections, we obtain the voltage dynamic associated with the changes of chemical species.

For illustration purposes, the fuel flow rate was set at 0.1 g s<sup>-1</sup> with a composition of 97% H<sub>2</sub> and 3% H<sub>2</sub>O, and set an air flow rate at 0.5 g s<sup>-1</sup>. Using the valve constants calculated in Section 2.1.2.3 and assuming the initial partial pressure of each gas is 1 atm, simulation results of gas partial pressures and the Nernst voltage generated across the stack are shown in Figs. 4 and 5, respectively. The time constant can be tens of seconds. The steady state cell voltage is around 1.046 V and drops to 0.97 V when the cell current increases from zero to 10 A. Note that the partial pressures of H<sub>2</sub> and H<sub>2</sub>O inside the SOFC stack are indeed at least two times higher than their ambient pressures. Therefore, the previous assumption on the choked orifice is valid. However,

for O<sub>2</sub>, the assumption may not hold for lower oxygen flows, when the stack current is high, as shown in the  $i = 10\text{ A}$  case.

2.1.2.8. Calculate the cell voltage. The total cell voltage can be represented as

$$V = V_{\text{Nernst}} + V_{\text{B,V}} + V_r + V_{\text{anode}} + V_{\text{cathode}} \quad (26)$$

where  $V_{\text{B,V}}$  is the Butler–Volmer over-potential resulting from charge transfer at low current,  $V_r$  the voltage drop caused by the material resistances, and  $V_{\text{anode}}$  and  $V_{\text{cathode}}$  are the over-potentials caused by diffusion in the cell anode and cathode. In the dynamic model, we assume that the  $V_{\text{B,V}}$  and  $V_r$  do not change with respect to the change of chemical species.  $V_{\text{anode}}$  and  $V_{\text{cathode}}$  are very small when the current is low; in other words, when the partial pressure of each gas is low. When the current increases, the  $V_{\text{anode}}$  and  $V_{\text{cathode}}$  start to dominate the cell output voltage. During the modeling, the partial pressures of each chemical species are used to calculate diffusion coefficients to account for the electrochemical dynamics in the cell reaction.

In the next section, we will briefly address the design considerations of an SOFC stack and then present our simulation results for a running SOFC stack, obtained by combining the thermal dynamic model discussed in Section 2.1.1 and the electrochemical dynamic model discussed in Section 2.1.2.

## 2.2. The combustor module

The combustor is mainly used in a standalone SOFC unit to supply extremely high temperature gas to the downstream heat exchanger. The high temperature gas is used to heat fuel and air inside the heat exchanger from their storage temperature to an appropriate temperature ready to be sent to the SOFC stack. Besides its main function, other benefits of the combustor

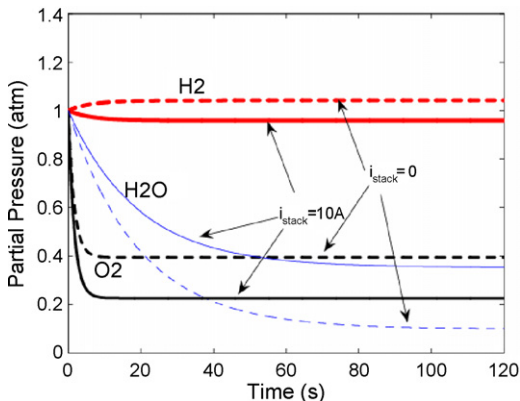


Fig. 4. The partial pressures of the H<sub>2</sub>, O<sub>2</sub>, and H<sub>2</sub>O.

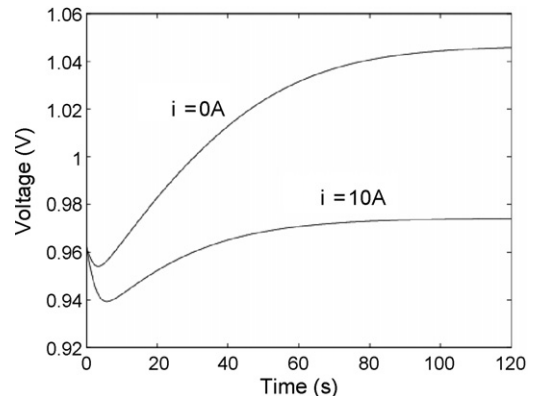


Fig. 5. The Nernst voltage in a cell.

include combusting the exhaust from the SOFC, recycling extra heat and preventing the exhaust of CO.

Three parameters of the outlet flow of the combustor are considered: the outlet flow rate ( $\text{g s}^{-1}$ ), the molar fraction of the outlet flow and the temperature of the outlet flow. The combustor model is explained in two parts in this section. The first part is the derivation of the outlet flow rate and its molar fraction. The second part is the calculation of the temperature of the outlet flow.

### 2.2.1. The outlet flow rate and its molar fraction

Assume that we know the inlet flow rate  $w^{\text{in}}$  ( $\text{g s}^{-1}$ ), inlet flow molar fraction ( $y_{\text{H}_2}^{\text{in}}, y_{\text{H}_2\text{O}}^{\text{in}}, y_{\text{O}_2}^{\text{in}}, y_{\text{N}_2}^{\text{in}}$ ), and inlet temperature  $T^{\text{in}}$  ( $^{\circ}\text{C}$ ). The molar flow rate of the inlet flow can be calculated by

$$n^{\text{in}} = \frac{w^{\text{in}}}{y_{\text{H}_2}^{\text{in}} M_{\text{H}_2} + y_{\text{H}_2\text{O}}^{\text{in}} M_{\text{H}_2\text{O}} + y_{\text{O}_2}^{\text{in}} M_{\text{O}_2} + y_{\text{N}_2}^{\text{in}} M_{\text{N}_2}} \quad (27)$$

The molar flow rate of each gas component is given by

$$n_i^{\text{in}} = n^{\text{in}} y_i^{\text{in}} \quad (28)$$

The reaction that happened in the combustor can be expressed as  $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$ . Because the SOFC stack and the combustor are always supplied with surplus air, it is reasonable to assume that 100% of the inlet hydrogen is combusted. Then we have the molar changes of each of the species after the reaction:

$$\begin{aligned} n_{\text{H}_2}^{\text{combusted}} &= n_{\text{H}_2}^{\text{in}}, & n_{\text{O}_2}^{\text{consumed}} &= 0.5n_{\text{H}_2}^{\text{in}}, \\ n_{\text{H}_2\text{O}}^{\text{generated}} &= n_{\text{H}_2}^{\text{in}} \end{aligned} \quad (29)$$

The outlet molar flow rate of each individual gas is

$$\begin{aligned} n_{\text{H}_2}^{\text{out}} &= n_{\text{H}_2}^{\text{in}} - n_{\text{H}_2}^{\text{combusted}} = 0, \\ n_{\text{O}_2}^{\text{out}} &= n_{\text{O}_2}^{\text{in}} - n_{\text{O}_2}^{\text{consumed}} = n_{\text{O}_2}^{\text{in}} - 0.5n_{\text{H}_2}^{\text{in}}, \\ n_{\text{H}_2\text{O}}^{\text{out}} &= n_{\text{H}_2\text{O}}^{\text{in}} + n_{\text{H}_2\text{O}}^{\text{generated}} = n_{\text{H}_2\text{O}}^{\text{in}} + n_{\text{H}_2}^{\text{in}}, \\ n_{\text{N}_2}^{\text{out}} &= n_{\text{N}_2}^{\text{in}} \end{aligned} \quad (30)$$

The total outlet molar flow rate is the summation of the molar flow rate of individual gases:

$$n^{\text{out}} = n_{\text{H}_2}^{\text{out}} + n_{\text{O}_2}^{\text{out}} + n_{\text{H}_2\text{O}}^{\text{out}} + n_{\text{N}_2}^{\text{out}} \quad (31)$$

The molar fraction of the outlet flow can be calculated by

$$y_i^{\text{out}} = \frac{n_i^{\text{out}}}{n^{\text{out}}} \quad (32)$$

Finally we get the mass flow rate ( $\text{g s}^{-1}$ ) of the outlet flow:

$$w^{\text{out}} = n_{\text{H}_2}^{\text{out}} M_{\text{H}_2} + n_{\text{O}_2}^{\text{out}} M_{\text{O}_2} + n_{\text{H}_2\text{O}}^{\text{out}} M_{\text{H}_2\text{O}} + n_{\text{N}_2}^{\text{out}} M_{\text{N}_2} \quad (33)$$

### 2.2.2. Temperature calculation of the outlet flow

Temperature calculation of the outlet flow is based on energy balance. The energy released from combustion is equal to the energy absorbed by the outlet gases. Using  $25^{\circ}\text{C}$  ( $298\text{ K}$ ) as a reference for potential heat energy, the potential heat energy of the outlet gas should be equal to the summation of the potential

Table 2  
Specific heat and enthalpy of the chemical species in the SOFC stack

Chemical species	Enthalpy of formation $\Delta H_f^{\circ}$ ( $\text{J mol}^{-1}$ )	$c_p$ ( $\text{J mol}^{-1} \text{K}^{-1}$ )
$\text{H}_2$	0	28.8
$\text{O}_2$	0	29.4
$\text{H}_2\text{O}(\text{l})$	-285.830	75.3
$\text{H}_2\text{O}(\text{g})$	-241.820	33.6
$\text{N}_2$	0	29.1

heat energy of the inlet gas and the energy released from the combustion of hydrogen. The energy balance of gases inside the combustor is then represented by

$$Q^{\text{out}} = Q^{\text{in}} + Q^{\text{com}} \quad (34)$$

where  $Q^{\text{com}}$  is the energy of combustion,  $Q^{\text{out}}$  the energy to heat the outlet gas from  $298\text{ K}$  to the outlet temperature, and  $Q^{\text{in}}$  is the energy to cool the inlet gas from the inlet temperature to  $298\text{ K}$ .

The energy needed to cool 1 mol of the inlet flow  $q$  to  $298\text{ K}$  can be calculated by

$$\begin{aligned} q_{\text{H}_2}^{\text{in}} &= c_p^{\text{H}_2}(T^{\text{in}} - 298), & q_{\text{O}_2}^{\text{in}} &= c_p^{\text{O}_2}(T^{\text{in}} - 298), \\ q_{\text{H}_2\text{O}}^{\text{in}} &= c_p^{\text{H}_2\text{O}(\text{l})}(373 - 298) + (\Delta H_{\text{f}(\text{H}_2\text{O},\text{g})}^{\circ} - \Delta H_{\text{f}(\text{H}_2\text{O},\text{l})}^{\circ}) \\ &\quad + c_p^{\text{H}_2\text{O}(\text{g})}(T^{\text{in}} - 373), \\ q_{\text{N}_2}^{\text{in}} &= c_p^{\text{N}_2}(T^{\text{in}} - 298) \end{aligned} \quad (35)$$

Note that the term  $(\Delta H_{\text{f}(\text{H}_2\text{O},\text{g})}^{\circ} - \Delta H_{\text{f}(\text{H}_2\text{O},\text{l})}^{\circ})$ , which equals  $44\,010\text{ J mol}^{-1}$ , appears in the equation as the energy needed to gasify the water, or the molar enthalpy of vaporization of water. Refer to Table 2 for the specific heat and enthalpy of the chemical species in an SOFC stack.

The energy carried by the inlet flow is given by

$$Q^{\text{in}} = n_{\text{H}_2}^{\text{in}} q_{\text{H}_2}^{\text{in}} + n_{\text{O}_2}^{\text{in}} q_{\text{O}_2}^{\text{in}} + n_{\text{H}_2\text{O}}^{\text{in}} q_{\text{H}_2\text{O}}^{\text{in}} + n_{\text{N}_2}^{\text{in}} q_{\text{N}_2}^{\text{in}} \quad (36)$$

The energy  $Q$  released by the combustion

$$Q^{\text{com}} = -(n_{\text{H}_2\text{O}}^{\text{gen}} \Delta H_{\text{f}(\text{H}_2\text{O},\text{l})}^{\circ} - n_{\text{H}_2}^{\text{com}} \Delta H_{\text{f}(\text{H}_2)}^{\circ} - n_{\text{O}_2}^{\text{com}} \Delta H_{\text{f}(\text{O}_2)}^{\circ}) \quad (37)$$

The energy carried by 1 mol of the outlet flow can be calculated by

$$\begin{aligned} q_{\text{H}_2}^{\text{out}} &= c_p^{\text{H}_2}(T^{\text{out}} - 298), & q_{\text{O}_2}^{\text{out}} &= c_p^{\text{O}_2}(T^{\text{out}} - 298), \\ q_{\text{H}_2\text{O}}^{\text{out}} &= c_p^{\text{H}_2\text{O}(\text{l})}(373 - 298) + 44\,010 + c_p^{\text{H}_2\text{O}(\text{g})}(T^{\text{out}} - 373), \\ q_{\text{N}_2}^{\text{out}} &= c_p^{\text{N}_2}(T^{\text{out}} - 298) \end{aligned} \quad (38)$$

The energy carried by the outlet flow is given by

$$Q^{\text{out}} = n_{\text{H}_2}^{\text{out}} q_{\text{H}_2}^{\text{out}} + n_{\text{O}_2}^{\text{out}} q_{\text{O}_2}^{\text{out}} + n_{\text{H}_2\text{O}}^{\text{out}} q_{\text{H}_2\text{O}}^{\text{out}} + n_{\text{N}_2}^{\text{out}} q_{\text{N}_2}^{\text{out}} \quad (39)$$

$T^{\text{out}}$  can then be calculated by solving the above equations.



### 2.3. The heat exchanger module

A heat exchanger is used in the SOFC unit to heat the inflow gases to an appropriate temperature using the heat generated by combustion of the inflow gases and the heat carried by the exhaust gases. Heat is transferred from the hot inlet flow to the cold inlet flow. There are two major concerns here in the modeling of a heat exchanger: the heat exchanging rate and the maximum heat that can be transferred. In the following discussion, annotation '1' stands for the hot flow, whereas annotation '2' represents the cold flow to be heated. The heat exchange process can be represented by

$$\begin{aligned} \rho_1 c_{p1} V_1 \frac{d}{dt} T_1^{\text{out}} &= \dot{Q}^{\text{in}} - \dot{Q}_1^{\text{out}} - \dot{Q}^{\text{transfer}}, \\ \rho_2 c_{p2} V_2 \frac{d}{dt} T_2^{\text{out}} &= \dot{Q}_2^{\text{in}} - \dot{Q}_2^{\text{out}} + \dot{Q}^{\text{transfer}} \end{aligned} \quad (40)$$

So we have

$$\begin{aligned} \rho_1 c_{p1} V_1 \frac{d}{dt} T_1^{\text{out}} &= w_1 c_{p1} (T_1^{\text{in}} - T_1^{\text{out}}) - \dot{Q}^{\text{transfer}}, \\ \rho_2 c_{p2} V_2 \frac{d}{dt} T_2^{\text{out}} &= w_2 c_{p2} (T_2^{\text{in}} - T_2^{\text{out}}) + \dot{Q}^{\text{transfer}} \end{aligned} \quad (41)$$

where  $w_i$  is the mass flow rate ( $\text{kg s}^{-1}$ ),  $c_{pi}$  the specific heat ( $\text{J kg}^{-1} \text{K}^{-1}$ ), and  $\dot{Q}_i$  is the heat.

The heat transfer effectiveness is defined as the actual heat transfer rate divided by the maximum possible heat transfer rate [19]:

$$\varepsilon = \frac{\dot{Q}^{\text{transfer}}}{\dot{Q}_{\text{max}}} \quad (42)$$

Let us assume the heat transferred between the two gases is a function of the inlet temperatures in the following form:

$$\dot{Q}^{\text{transfer}} = k_q (T_1^{\text{in}} - T_2^{\text{in}}) \quad (43)$$

Then the heat exchange rate rises to its maximum value when  $k_q$  takes its maximum value

$$\dot{Q}_{\text{max}} = k_q^{(\text{max})} (T_1^{\text{in}} - T_2^{\text{in}}) \quad (44)$$

The maximum heat exchange rate happens when the outlet temperatures of the two gases are equal. Solving the differential equations, the outlet temperatures can be expressed as functions of time

$$\begin{aligned} T_1^{\text{out}}(t) &= \frac{w_1 c_{p1} - k_q}{w_1 c_{p1}} T_1^{\text{in}} + \frac{k_q}{w_1 c_{p1}} T_2^{\text{in}} - \left( T_1^{\text{in}} + \frac{w_1 c_{p1} - k_q}{w_1 c_{p1}} T_1^{\text{in}} + \frac{k_q}{w_1 c_{p1}} T_2^{\text{in}} \right) e^{(-w_1 c_{p1} / \rho_1 c_{p1} V_1) t}, \\ T_2^{\text{out}}(t) &= \frac{w_2 c_{p2} - k_q}{w_2 c_{p2}} T_2^{\text{in}} + \frac{k_q}{w_2 c_{p2}} T_1^{\text{in}} - \left( T_2^{\text{in}} + \frac{w_2 c_{p2} - k_q}{w_2 c_{p2}} T_2^{\text{in}} + \frac{k_q}{w_2 c_{p2}} T_1^{\text{in}} \right) e^{(-w_2 c_{p2} / \rho_2 c_{p2} V_2) t} \end{aligned} \quad (45)$$

The steady state solution of the differential equation is

$$\begin{aligned} T_1^{\text{out}} &= \frac{w_1 c_{p1} - k_q}{w_1 c_{p1}} T_1^{\text{in}} + \frac{k_q}{w_1 c_{p1}} T_2^{\text{in}}, \\ T_2^{\text{out}} &= \frac{w_2 c_{p2} - k_q}{w_2 c_{p2}} T_2^{\text{in}} + \frac{k_q}{w_2 c_{p2}} T_1^{\text{in}} \end{aligned} \quad (46)$$

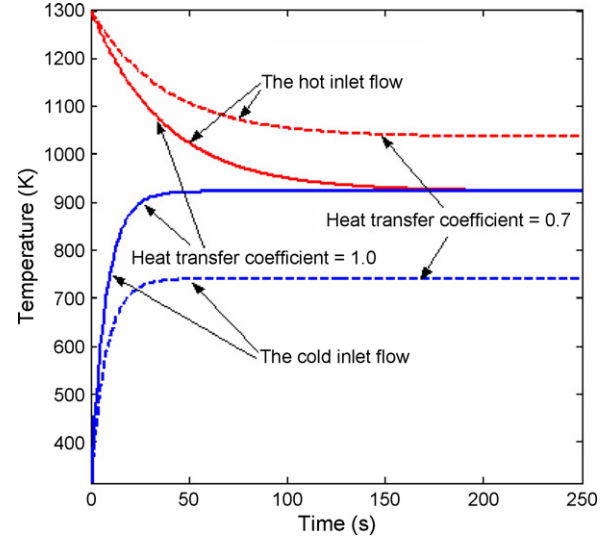


Fig. 6. An example of the calculation results of the heat exchanger model.

When  $T_1^{\text{out}}$  equals  $T_2^{\text{out}}$ , the maximum heat exchange rate happens and  $k_q$  takes its maximum value:

$$k_q^{(\text{max})} = \frac{w_1 c_{p1} w_2 c_{p2}}{w_1 c_{p1} + w_2 c_{p2}} \quad (47)$$

So,

$$\dot{Q}_{\text{max}} = \frac{w_1 c_{p1} w_2 c_{p2}}{w_1 c_{p1} + w_2 c_{p2}} (T_1^{\text{in}} - T_2^{\text{in}}) \quad (48)$$

$$\text{Let } C_{\text{min}} = \frac{w_1 c_{p1} w_2 c_{p2}}{w_1 c_{p1} + w_2 c_{p2}},$$

We get

$$\begin{aligned} \rho_1 c_{p1} V_1 \frac{d}{dt} T_1^{\text{out}} &= w_1 c_{p1} (T_1^{\text{in}} - T_1^{\text{out}}) - \varepsilon C_{\text{min}} (T_1^{\text{in}} - T_2^{\text{in}}), \\ \rho_2 c_{p2} V_2 \frac{d}{dt} T_2^{\text{out}} &= w_2 c_{p2} (T_2^{\text{in}} - T_2^{\text{out}}) + \varepsilon C_{\text{min}} (T_1^{\text{in}} - T_2^{\text{in}}) \end{aligned} \quad (49)$$

Fig. 6 shows an example of the calculation results of the heat exchanger model when the heat transfer coefficient is equal to 0.7 and 1.0, respectively. The temperature of the hot inlet flow is 1300 K in the example, whereas the temperature of the cold inlet flow is 315 K. The calculation results show that when heat transfer coefficient is equal to 1.0, the outlet temperatures

of both flows are equal. Based on the above equations, the state space representation of the partial pressure model is then written as

$$\dot{X} = AX + Bu, \quad Y = CX + Du \quad (50)$$

where

$$X = \begin{bmatrix} T_1^{\text{out}} \\ T_2^{\text{out}} \end{bmatrix}, \quad u = \begin{bmatrix} T_1^{\text{in}} \\ T_2^{\text{in}} \end{bmatrix}, \quad A = \begin{bmatrix} -\frac{w_1}{\rho_1 V_1} & 0 \\ 0 & -\frac{w_2}{\rho_2 V_2} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{w_1 c_{p1} - \varepsilon C_{\text{min}}}{\rho_1 c_{p1} V_1} & \frac{\varepsilon C_{\text{min}}}{\rho_1 c_{p1} V_1} \\ \frac{\varepsilon C_{\text{min}}}{\rho_2 c_{p2} V_2} & \frac{w_2 c_{p2} - \varepsilon C_{\text{min}}}{\rho_2 c_{p2} V_2} \end{bmatrix},$$

$$C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

2.4. The simulation results of an SOFC APU at running mode

In the controller design for an SOFC stack, there should be three control objectives: temperature, voltage and fuel utilization. The following constraints have to be met:

- (A) The stack temperature will not exceed its upper and lower temperature limits.
- (B) The voltage should be managed to be above its lower limit while A is satisfied.
- (C) The fuel utilization should be above its lower limit provided that (A) and (B) are satisfied.

Because it is not the focus of this paper to discuss the control scheme of the SOFC APU, a simplified controller model is chosen. It consists of two parts: the control of the fuel utilization and the control of the heat exchanger flow mix. With the controller, one can control the fuel and air flow rates and temperatures.

Using MATLAB, we implemented the above thermal dynamic and electrochemical dynamic models to simulate an SOFC stack containing 60 cells at operation mode. The load is purely resistive. At 5 s, the load changes from 60 to 3 Ω. As shown in Fig. 7, the voltage then drops from 60 to 41.3 V. If we set the fuel flow to ramp up at 0.04 g s<sup>-1</sup> from 15 to 20 s, as shown in Fig. 8, we have the voltage and current increase accordingly. However, the fuel utilization will drop significantly from 0.55 down to 0.06.

From the simulation results shown in Figs. 7 and 8, we have the following observations:

- Different dynamics have different time constants. As shown in Fig. 7, the stack temperature will not change significantly during tens of seconds; therefore, thermal dynamics will not in general affect the electric dynamic responses, which happen in a few seconds at the most. Electrochemical dynamics are within seconds and may interact with the electric dynamics caused by outside circuits. The fluid dynamics may happen in seconds because of the fan, valves, and the inlet and outlet parameters.
- When fuel flow rates increase, one can boost the stack voltage and current in seconds. However, the fuel utilization will

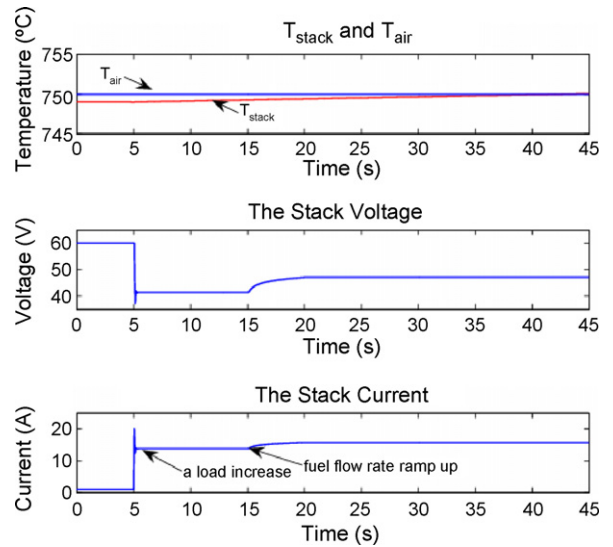


Fig. 7. The stack temperatures, voltage, and current.

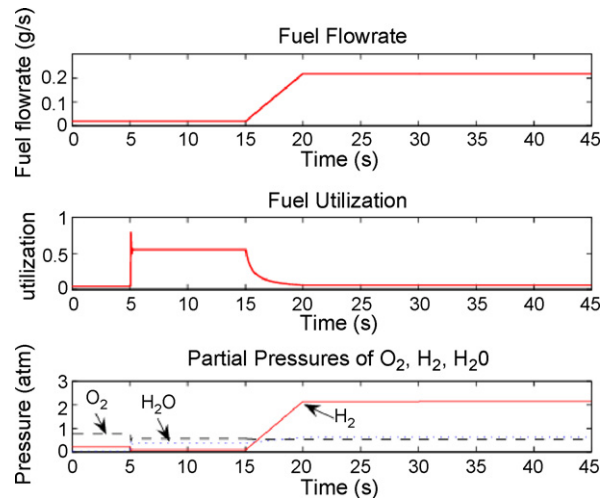


Fig. 8. The fuel flow rate, the fuel utilization, and partial pressures of an SOFC stack.

drop sharply, and the pressure inside the SOFC stack will increase as well, causing low efficiency and high mechanical stresses inside the SOFC, both of which are not desired. Furthermore, the rise in voltage is not significant when fuel flow rate increases further. Therefore, the voltage regulation of the SOFC is very limited.

3. Conclusions

This paper has addressed the dynamic modeling issues in modeling a standalone SOFC auxiliary power unit. While providing greater accuracy, detailed SOFC models such as CFD take considerable computer resources to run, and it is inconvenient to couple detailed models with an electric circuit model to simulate the electric circuit dynamic response. An objective of this research has been to set up lumped thermal dynamic and electrochemical dynamic models to improve the computational

time and provide reasonable accuracy of the calculated stack voltage, temperature, and fuel utilization. Detailed derivation of model parameters has been presented. The constraints and parameters of the lumped model have been obtained through detailed models and experimental data. This SOFC dynamic model is expected to be used for SOFC controller design as well as simulating the dynamic response of SOFC in power systems.

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### References

- [1] K.P. Recknagle, R.E. Williford, L.A. Chick, D.R. Rector, M.A. Khaleel, Three-dimensional thermo-fluid electrochemical modeling of planar SOFC stacks, *J. Power Sources* 113 (2002) 109–114.
- [2] J.T. Pukrushpan, H. Peng, A.G. Stefanopoulou, Simulation and analysis of transient fuel cell system performance based on a dynamic reactant flow model, in: *Proceedings of the IMECE'02*, New Orleans, LA, USA, 2002.
- [3] R.F. Mann, J.C. Amphlett, M.A.I. Hooper, H.M. Jensen, B.A. Peppley, P.R. Roberge, Development and application of a generalized steady-state electrochemical model for a PEM fuel cell, *J. Power Sources* 86 (2000) 173–180.
- [4] E. Achenbach, Response of a solid oxide fuel cell to load change, *J. Power Sources* 57 (1995) 105–109.
- [5] M.Y. El-Sharkh, A. Rahman, M.S. Alam, A.A. Sakla, P.C. Byrne, T. Thomas, Analysis of active and reactive power control of a stand-alone PEM fuel cell power plant, *IEEE Trans. Power Syst.* 19 (4) (2004) 2022–2028.
- [6] M.D. Lukas, K.Y. Lee, H. Ghezal-Ayagh, Development of a stack simulation model for control study on direct reforming molten carbonate fuel cell power plant, *IEEE Trans. Energy Convers.* 14 (4.) (1999).
- [7] J. Padullés, G.W. Ault, J.R. McDonald, An integrated SOFC plant dynamic model for power system simulation, *J. Power Sources* 86 (2000) 495–500.
- [8] M.D. Lukas, K.Y. Lee, H. Ghezal-Ayagh, Development of a stack simulation model for control study on direct reforming molten carbonate fuel cell power plant, *IEEE Trans. Energy Convers.* 14 (1999) 1651–1657.
- [9] J.C. Amphlett, R.M. Baumert, R.F. Mann, B.A. Peppley, P.R. Roberge, A. Rodrigues, Parametric modeling of the performance of a 5 kW proton-exchange membrane fuel cell stack, *J. Power Sources* 49 (1994) 349–356.
- [10] S.I. Sandler, *Chemical Engineering Thermodynamics*, John Wiley & Sons, New York, 1989.
- [11] Perry's *Chemical Engineers' Handbook*, 7th ed., McGraw-Hill Co., 1997.
- [12] M.R. Beychok, February 27, 2006. <http://www.air-dispersion.com/msource.html>.
- [13] *Handbook of Chemical Hazard Analysis Procedures* Federal Emergency Management Agency, U.S. Dept. of Transportation and U.S. Environmental Protection Agency, 1989.
- [14] H.J. Clewell, A Simple Method for Estimating the Source Strength of Spills of Toxic Liquids, Energy Systems Laboratory, ESL-TR-83-03, 1983. Available at Air Force Weather Technical Library, Asheville, NC.
- [15] G. Ille, C. Springer, The Evaporation And Dispersion Of Hydrazine Propellants From Ground Spills, Civil and Environmental Engineering Development Office, CEEDO 712-78-30, 1978. Available at Air Force Weather Technical Library, Asheville, NC.
- [16] J.P. Kahler, R.C. Curry, R.A. Kandler, Calculating Toxic Corridors, Air Force Weather Service, AWS TR-80/003, 1980. Available at Air Force Weather Technical Library, Asheville, NC.
- [17] M.J. Moran, H.N. Shapiro, B.R. Munson, D.P. Dewitt, *Introduction to Thermal Systems Engineering: Thermodynamics, Fluid Mechanics and Heat Transfer*, John Wiley & Sons, New York, 2003, pp. 535–537.
- [18] *CRC Handbook of Chemistry and Physics*, February 27, 2006. <http://www.hbcpnetbase.com/>.
- [19] *ASHRAE Handbook*, 1985 Fundamentals, SI-Edition, ASHRAE, Inc., Atlanta, GA, 1985.