Dynamic Modeling of a Solid Oxide Fuel Cell System for Control Design

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Abstract—Solid Oxide Fuel Cell (SOFC) power systems are under active development for a range of applications. Tight thermo-chemical operating constraints together with strong thermal coupling in SOFC systems present significant challenges for system and control design. To facilitate model-based system design addressing steady state and transient performance requirements, first principles based component and system dynamic models are developed for a compact SOFC system. The models are partially validated using some experimental data. The dynamic interactions in the system relevant to fuel cell stack thermal management and system control design are discussed using open-loop model simulations.

I. INTRODUCTION

Fuel cells can directly convert chemical energy to electricity using electrochemical reactions and have higher efficiency than conventional, combustion based power systems. The higher efficiency coupled with reduction in harmful emissions make them environmentally friendly power sources. Solid Oxide Fuel Cell (SOFC) systems use a ceramic electrolyte based fuel cell and operate at high temperatures (>600°C). They are fuel-flexible and are particularly attractive for stationary and mobile applications [1]–[3].

For mobile applications, SOFC systems to provide either auxiliary power or main propulsion power are under development. For instance, SOFC based Auxiliary Power Units (APU) are being developed and tested for heavy-duty trucks to provide electrical power to auxiliary devices [4]. Using SOFC APUs can significantly decrease the time of the inefficient engine operation (e.g. idling), thus reducing fuel costs and emissions [5]. SOFC technology is also a promising clean and efficient power solution for marine applications [2], [6]. For example, the U.S. Office of Naval Research has initiated a program to demonstrate a ship service fuel cell power system to improve efficiency and sustainability of vessels [7], [8]. The U.S. Naval Undersea Warfare Center has also been developing SOFC technology for Unmanned Underwater Vehicles (UUV) in order to greatly increase endurance of UUV missions [9].

Although SOFC technology has been evolving rapidly in recent years, many technical challenges, including material stability, component fabrication, system design and control, need to be addressed before large-scale commercialization can be achieved [3]. In mobile applications, the power system is subject to relatively large and rapid changes in electrical loads, necessitating more emphasis on system transient performance. SOFC systems, however, are known to have slow power transient capability due to large thermal inertia [10]. Due to the high operating temperature of SOFC systems, effective thermal management is essential to providing the desired system performance while ensuring operational safety and component durability. For example, both the maximum temperature and the maximum temperature gradient in the cell must be constrained at steady-state and during transients, in order to ensure material stability and avoid thermal cracking [3], [11]. In addition, compared to stationary applications, the size and weight requirements for the power system in mobile applications are more stringent. This requires a compact and well-integrated SOFC system which inevitably has strong coupling among different components.

Model based design methodology has long been recognized as effective for the development of SOFC technology, including component and system design as well as control design. While substantial efforts were made on SOFC component level modeling [12], [13], the research that addresses system level dynamic modeling and control design for SOFC systems is sparse. Existing literature focuses on SOFC-Gas Turbine systems [14]–[17]. The literature on mobile SOFC system dynamic modeling and control design is limited. In [18], a dynamic model was developed for mobile SOFC APU systems without an after-burner and air-preheater and used for steady-state and dynamic system analysis as well as control design to improve the system transient performance. Dynamic models for SOFC and steam reformer based systems were developed and control algorithms for fast load following were proposed in [19], [20]. In [21], a planar SOFC based automotive APU was modeled and the system performance was analyzed without providing a detailed model description. In [22], a simplified thermodynamic model was derived for a mobile SOFC system to study system thermal behavior and operational strategy. The influence of the power conditioning system on the operation performance of the SOFC and Balance-of-Plant (BOP) components was investigated using system model simulations in [23]. In [24], control-oriented dynamic models for transient analysis of SOFC systems were presented. It should be noted that most of the dynamic models available in literature had not been validated against experimental data, mainly due to the limited availability of test data.

In this paper, we develop component and system dynamic models for a compact SOFC system to facilitate transient analysis and control design. The SOFC system considered is suitable for mobile applications. Physics-based component
models are formulated as differential-algebraic equations and implemented in an equation-oriented modeling tool, gPROMS\textsuperscript{TM} [25]. A system model is then assembled from the component models. The component models are validated against limited experimental data available from a prototype unit that is under development at UTRC. The system model is further calibrated to match the system test results. It was found that models capture proper trends during transients, although additional parameter tuning and model refinement may be needed to improve the quantitative accuracy. The dynamic characteristics of the system, particularly relating to the SOFC stack thermal management are discussed using open loop system model simulations.

The rest of the paper is organized as follows: A brief description of the SOFC system considered is given in Section II. Physics-based component and system dynamic models are described in Section III. In Section IV, model validation with experimental data is presented. Open loop simulation results are presented and implications to stack thermal management and system control are discussed in Section V. Conclusions are presented in Section VI.

II. SYSTEM DESCRIPTION

Figure 1 shows the configuration of a SOFC system considered in this paper. In this system, the hydrocarbon fuel is first processed in a Catalytic Partial Oxidation (CPO) reformer and converted into a mixture mainly consisting of $H_2$, $H_2O$, $CO$, $CO_2$ and $N_2$. The reformate is then fed into the fuel channels of the planar SOFC stack where the fuel is consumed to generate electricity through the electrochemical reaction. On the air side, fresh air is pre-heated in the heat recovery unit (i.e., the recuperator) and then sent to the CPO reformer for fuel processing and the stack for electrochemical reaction and stack cooling. After the stack, the remaining fuel in the anode exhaust is mixed with the cathode outlet and combusted in the Catalytic Burner (CB). The high temperature burner exhaust flows into the recuperator to heat up the air inlet. In next section, dynamic models of these components and the entire system are described.

III. DYNAMIC MODELING

As described below, first-principle dynamic models are first developed for all the components shown in Fig. 1, based on which a SOFC system dynamic model is then assembled.

A. SOFC Stack

A physics-based lumped parameter stack model is developed to describe the key dynamics of the SOFC stack. The stack model includes three major components: mass balance, energy balance and electrochemical characteristics. To make the stack model more generic and applicable for other system study, internal reforming reactions are also incorporated. Therefore, the following four reactions are considered in the model:

- Steam reforming (SR) $\text{CH}_4 + H_2O \rightarrow CO + 3H_2$
- Water gas shift (WGS) $CO + H_2O \rightarrow CO_2 + H_2$
- Oxidation (Ox) $H_2 + O^2- \rightarrow H_2O + 2e^-$
- Reduction (Red) $0.5O_2 + 2e^- \rightarrow O^2-.$

The mass balance dynamics of the fuel and air flows in the fuel cell gas channels can be described as follows:

\[
\begin{align*}
\text{fuel} : \dot{m}_{f,s}^a &= W_{f, in,s}^a - W_{f, out,s}^a + \sum_{k \in \{SR,WGS,OX\}} \nu_{s,k} r_k M_{s,k} \\
\text{air} : \dot{m}_{a,s}^a &= W_{a, in,s}^a - W_{a, out,s}^a + \nu_{a, Red} r_{Red} M_{a,s} 
\end{align*}
\]

where $m_{f,s}^a$ and $m_{a,s}^a$ are the mass holdup of species $s$ in the fuel channel and species $s$ in the air channel, respectively, $W_{f, in,s}^a$ and $W_{f, out,s}^a$ are the inlet and outlet mass flowrates of species $s$ in the fuel stream, respectively, and $W_{a, in,s}^a$ and $W_{a, out,s}^a$ are for the air stream. $\nu_{s,k}$ is the stoichiometric coefficient of species $s$ in reaction $k$ and $r_k$ the reaction rate of reaction $k$. $M_{s,f}$ and $M_{s,a}$ are the molar mass of species $s$ in the fuel channel and species $s$ in the air channel, respectively.

The reaction rate, $r_k$, is calculated as follows:

\[
\begin{align*}
\dot{r}_{OX} &= r_{Red} = \frac{i}{2F} \\
\dot{r}_{SR} &= 0.04274p_{CH_4} \exp\left(\frac{-8200}{RT_f}\right) \\
\dot{r}_{WGS} &= k_{WGS} p_{CO} \left(1 - \frac{p_{CO_2} p_{H_2}}{p_{CO} p_{H_2} \kappa_{eq,WGS}}\right)
\end{align*}
\]

where $i$ is the current density, $F$ Faraday constant, $p_s$ the partial pressure of species $s$, $T_f$ the fuel channel temperature, $R$ the ideal gas constant, $k_{WGS}$ the constant coefficient and $\kappa_{eq,WGS}$ the temperature dependent equilibrium constant of WGS reaction. Eqn. (3) comes from the Faraday’s law. The formula described in Eqn. (4) is widely used in the literature [26]–[28]. Eqn. (5) is adopted in [27], where $k_{WGS}$ assumes large value, reflecting the very fast kinetics of the WGS reaction.

Three temperature layers are assumed in a single cell, namely the fuel flow, air flow and solid structure. The energy balance dynamics of the fuel and air stream as well as the solid structure are described as follows:

\[
\begin{align*}
\text{fuel} : \dot{E}_f &= H_f^f - H_f^i - H_{f,s}^a - Q_{f,s}^a - Q_{f, loss}^a \\
\text{air} : \dot{E}_a &= H_a^a - H_a^i - H_{a,s}^a - Q_{a,s}^a - Q_{a, loss}^a \\
\text{solid} : m_{s,p,s} \dot{T}_s &= H_{s,s}^f + H_{s,a}^a + Q_{s,s}^f + Q_{s,a}^a - VI - Q_{s, loss}^a
\end{align*}
\]
where $E_f$ and $E_a$ are the energy holdup in the fuel and air flow channels, respectively. $H_{in}^f$ and $H_{out}^f$ are the enthalpy flowrate of the fuel inlet and outlet in the stack. $H_{in}^{f_{OS}}$ is the net enthalpy flowrate associated with the mass transport from the fuel stream to the catalyst. $Q_{in}^{f_{OS}}$ is the convective heat transfer between the fuel bulk flow and its surrounding wall. Similar to that with the superscript of “o” are used for the air stream. $T_s$ is the temperature in the solid structure. $m_s$ and $c_p,s$ are the mass and specific heat capacity of the solid structure in the stack. $V$ and $I$ are the stack voltage and current, respectively. $Q_{loss}$ is the heat loss from the stack.

By applying the electrochemical principle, the operating cell voltage can be calculated as follows:

$$V = V_{OCV} - (\eta_{ohm} + \eta_{act} + \eta_{ion})$$

where the last three terms are various potential losses, such as ohmic loss ($\eta_{ohm}$), activation loss ($\eta_{act}$) and concentration loss ($\eta_{ion}$). $V_{OCV}$ is the open circuit voltage determined by the Nernst equation as a function of stack temperature and gas composition. The voltage loss calculation follows standard expression in [1], [3] as follows:

$$\eta_{ohm} = i R_{ohm}(T),$$

$$\eta_{act} = \frac{RT}{\alpha F} \sinh^{-1} \left( \frac{i}{2i_0(T)} \right),$$

$$\eta_{ion} = a \exp(bt),$$

where $A$ is the active area of the cell, $R_{ohm}(T)$ the cell electrical resistance as a function of stack temperature, $\alpha$ is a constant coefficient and $i_0(T)$ the temperature dependent exchange current density. $a$ and $b$ are constant coefficients for each concentration loss. $R_{ohm}(T)$, $i_0(T)$, $\alpha$, $a$ and $b$ are obtained by curve-fitting experimental data. Some empirical relations either from the vendor or the test data are implemented as well to account for the influence of the spatial distributions of the temperature and gas composition along the flow path in the stack.

B. Catalytic Burner

The CB is also modeled as a lumped system and the following equations describe its key dynamics.

Mass balance:

$$\dot{m}_{cb}^{s} = W_{in,s}^{cb} - W_{out,s}^{cb} + \sum_{k \in \{cb \text{ reaction}\}} \nu_{s,k} r_k M_s$$

where $m_{cb}^{s}$ is the mass holdup of species $s$ in the CB chamber. $W_{in,s}^{cb}$ and $W_{out,s}^{cb}$ are the inlet and outlet mass flowrate of species $s$ in the stream, respectively. $\nu_{s,k}$ is the stoichiometric coefficient of species $s$ in reaction $k$ and $r_k$ the reaction rate of reaction $k$. Complete oxidation reactions are assumed for the fuel species remained in the CB inlet. $M_s$ is the molar mass of species $s$.

Similar to the energy balance in the SOFC stack model, the following dynamic energy balance equations can be derived for the gas stream and the solid part in the CB.

$$\text{gas}: \quad \dot{E}_{cb}^{s} = H_{in}^{cb} - H_{out}^{cb} - H_{toS}^{cb} - Q_{toS}^{cb}$$

$$\text{solid}: \quad \dot{m}_{cb}^{s} c_{p,s} T_s^{cb} = H_{toS}^{cb} + Q_{toS}^{cb} - Q_{loss}^{cb}$$

where $E_{cb}^{s}$ is the energy holdup in CB's gas chamber. $H_{in}^{cb}$ and $H_{out}^{cb}$ are the enthalpy flowrate of the inlet and outlet of the CB, respectively. $H_{toS}^{cb}$ is the net enthalpy flowrate associated with the mass transport from the gas stream to the catalyst. $Q_{toS}^{cb}$ is the convective heat transfer between the bulk flow and its surrounding solid parts. $T_s^{cb}$ is the temperature in CB's solid structure. $m_{cb}^{s}$ and $c_{p,s}$ are the mass and specific heat capacity of the solid part in CB. $Q_{loss}^{cb}$ is the heat loss to the environment.

By applying same thermodynamic principles and modeling approach, first-principle dynamic models are also developed for other BOP components, such as the CPO reformer, heat exchanger, air compressor and fuel pump. Based on these component models, a dynamic model is then assembled for the SOFC system described in Fig. 1. A lumped control volume model is also derived for the hot box that encloses the stack, reformer, heat exchanger and burner. Radiative and convective heat transfer among these components and the hot box are considered and incorporated in the system model. These models, modularized for reusability, are implemented in gPROMSTM, an equation-based modeling tool [25].

IV. MODEL VALIDATION

The component dynamic models were calibrated against some experimental data obtained from a prototype unit under development. Figure 2 illustrates the approach adopted for component model validation. Design information such as the geometry and material properties, as well as certain test data such as inlet flow rate, temperature and gas composition, were given to the model. Unknown parameters such as the heat transfer coefficients were then estimated to provide the best match between the model outputs and the experimental data. The validation setup was also implemented in gPROMSTM which provides a parameter estimation feature. Depending on the availability of test data, most of the component models were validated and an overall accuracy of 10–15% was achieved.
in the hotbox. The air and fuel inlets of the burner were pre-heated through the recuperator. The inlet temperature, composition, and outlet temperature of the burner were measured or calculated as inputs to the parameter estimation process. Two parameters were estimated: the coefficient of the convective heat transfer between the gas flow and the solid wall, and the heat transfer coefficient of the convective heat loss from the burner surface to the hot box. Given the operating conditions (e.g., fuel and air inlet flow rate, temperature and composition), these two parameters were optimized to match the outlet temperature at the burner exit within 1% error. Relatively larger discrepancy is observed during start-up mainly due to the unmodeled secondary effects, unexpected disturbance in the test as well as model initialization. However, only the operation near the nominal condition is of our primary interest for this study. To validate the results, the burner model with the same parameters was simulated for the operation conditions used in the second experiment. The comparison showed that the predicted outlet temperature was within 5% of the test data. Fig. 3 and the following figures in this paper show normalized numbers since the actual data is proprietary information.

![Fig. 3. Parameter estimation of CB model based on Experiment 1 data.](image)

After the component model validation, the system dynamic model was also tuned to match the system test data. In a system test run, fuel flow rate, CPO air flow rate, cathode air flow rate and stack current load were considered as inputs and varied as shown in Figure 5. The same input trajectories were applied to the system dynamic model and the simulation results for various output signals were then compared with the experimental data in Fig. 6. The comparisons for stack voltage, gross power output, the outlet temperature of CB and cathode as well as the temperature increase across the cathode are shown in Fig. 6. A reasonable match in the trends was observed from the comparison. The error in the stack voltage prediction seemed to be larger at higher power levels which suggests the need for further tuning of the cell performance model. The variations in the cathode outlet temperature and temperature difference were smaller than those presented in the test data. Their transients, however, exhibited correct trends compared to the test data.

![Fig. 5. System inputs in experiment. (y-axis numbers normalized)](image)

V. DYNAMIC ANALYSIS

It is important to obtain a good understanding of the system dynamic characteristics, such as the open-loop response trends, system coupling, nonlinearity and control authority, in order to design an effective control strategy. Using the dynamic system model described above, transient performance of the SOFC system can be investigated. As mentioned earlier, the maximum temperature and temperature gradient in the stack have to be kept below certain limits during the operation to ensure stack safety. In many practical applications, the maximum temperature is usually approximated by the cathode outlet temperature and the temperature difference.
across the cathode is monitored to reflect the temperature gradient in the stack. In this section, the open-loop system response is analyzed to study the dynamic performance of the cathode temperature during transient.

In Fig. 7, step response of the cathode inlet ($T_{\text{in}}^C$) and outlet temperature ($T_{\text{out}}^C$) as well as the temperature difference ($dT_c$) are shown where a 5% current increase is applied to the stack. It can be found that $T_{\text{out}}^C$ increases due to more heat produced by the electrochemical reaction. $T_{\text{in}}^C$, however, drops because, with higher current load and constant fuel supply, less fuel remains in the anode outlet, causing lower burner temperature and less heat available in the recuperator to pre-heat the cathode inlet. As a result, $dT_c$ increases.

Figure 8 shows the cathode temperature response to 5% fuel flow rate increase where $dT_c$ drops at the beginning of the transient and then grows but approaches to a level still below the original one. This may be used to compensate the increased $dT_c$ when the current is increased. The complementary effect is mainly due to the higher $T_{\text{in}}^C$ because of more fuel available in the anode exhaust and consequently more energy in the heat recuperator. Increasing the fuel inlet also helps reduce $T_{\text{out}}^C$ at the beginning, but leads to a higher $T_{\text{out}}^C$ at steady state which should be avoided.

Cathode air stream is generally considered as the main control mechanism for stack thermal management. To illustrate its impact, Fig. 9 gives the open-loop response of the cathode temperature when the air flow rate increases by 25%. After a short fluctuation at the beginning, $T_{\text{out}}^C$ gradually decrease and approach a lower steady-state temperature, showing the beneficial influence of the cathode air flow on controlling the maximum stack temperature. Larger air flowrate can bring more heat out of the stack. However, it shows little cooling effect on $dT_c$ in the system under study. In fact, $dT_c$ sees a considerable increase at the beginning of the transient because $T_{\text{in}}^C$ drops more quickly than $T_{\text{out}}^C$.

The above analysis indicates complex dynamic coupling in the system which must be taken into account when designing the control system. Both $T_{\text{out}}^C$ and $dT_c$ increases when SOFC system tries to follow the load increase. The fuel and air inlet flow rates have strong impact on the transient and steady-state behavior of the cathode temperature.

VI. CONCLUSION AND FUTURE WORK

First-principle dynamic models were developed for a SOFC system to facilitate system dynamic analysis and control design. Certain unknown parameters were estimated and the models were validated against experimental data. Open-loop response was analyzed to characterize the system dynamics and interactions relevant to stack thermal management. Future work will involve further model validation and
Fig. 9. Open loop response of cathode temperature to 25% increase of cathode air inlet flow rate.

refinement to improve accuracy and feedback control design using the developed models.

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