Solid Oxide Fuel Cell: Perspective of Dynamic Modeling and Control

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Abstract: This paper presents a review of state-of-the-art solid oxide fuel cells (SOFC), from perspective of dynamic modeling and model-based control. First, the current status of SOFC development is provided. Then the main components of the SOFC along with their governing transport equations are discussed. These two sections provide basic introduction to the SOFC. Following the sequence of power generation and energy losses mechanism of SOFC, the section of dynamic modeling is started from overview of energy generation, followed by discussion of energy losses, and concluded by analyzing the dynamics that affect energy generation and losses. The section of dynamic modeling is closed by considering the model validation problem and other related problems in the modeling aspect. Once dynamic models are available, the paper continues its journey to the SOFC control problems. It is started from a general description of the control problems in SOFC, continued with an overview of the existing control strategies, and followed by a sample nonlinear MPC solution. This section is concluded by discussion of some of the challenges in SOFC control problems.

Keywords: Solid Oxide Fuel Cell, Control Relevant Model, Model Predictive Control

1. INTRODUCTION

Today’s energy hungry civilization is in search of an alternative source to replace the currently available but continuously depleting energy sources. Stringent environmental regulations restricting emissions of greenhouse gases, SOx, and NOx have narrowed down the search for a clean source of energy to a few options. It has generated a lot of attention towards the fuel cell as one of the alternative sources of clean energy. Fuel cells are electrochemical devices that directly convert chemical energy to electrical energy. Since it does not involve any rotary or thermal components, it does not suffer from any friction and combustion loss. Moreover, the unused fuel from the cell can be used to generate more power, making it potentially high overall efficiency.

Among various fuel cells, the low temperature proton exchange membrane fuel cell (PEM) and the high temperature solid oxide fuel cell (SOFC) have been identified as the likely fuel cell technologies that may capture the most significant fuel cell market in the future. This paper will focus on SOFC.

In order to operate SOFC, it is necessary to understand its dynamic characteristics and then hopefully to control it optimally. Modeling and control are two integral parts of the advanced process control strategies which are intricately dependent on each other. From the view point of process control, the models should be easy to use for designing controllers and yet be detailed enough for giving a sufficient account of the system dynamics.

With the advent of cheap computational power, a surge of application of previously non-implementable complex controllers such as the nonlinear model predictive controller has been seen in industries. In this paper, nonlinear MPC is used to demonstrate control application in the fuel cell system, based on the models developed from first principles.

Dynamic models can be used to investigate responses of the fuel cells under different operating conditions to account for the pitfalls associated with the design and material selections. By means of optimal control, one can steer the operating condition towards favorable one to improve durability and efficiency of the fuel cells. On the other hand, a real-time monitoring system can safeguard fuel cell operations. Thus dynamic modeling, control and monitoring are the essential ingredients of fuel cell developments, and call for solutions and active participation from the process control community.

This paper will review the state-of-the-art SOFC from perspective of operation principles, dynamic modeling, and control strategies, developed by the authors as well as other researchers, over the recent years. Some of the challenges in the solid oxide fuel cell research will also be discussed.

2. STATE OF THE ART

Fuel cell is a well known alternative energy technology. It is also a highly efficient power generation technology. Conventionally, energy generation follows the route of combustion → producing heat → converting to kinetic energy → converting to electrical energy. The overall energy conversion efficiency is low. Fuel cells convert
chemical energy of fuel and oxidant directly into electrical energy through electrochemical reactions. Therefore the efficiency of a fuel cell power plant can be as high as 70% (Larminie and Dicks, 2003).

Depending on electrolytes, Alkaline fuel cell (AFC), Proton Exchange Membrane Fuel Cell (PEM), Direct Methanol Fuel Cell (DMFC), Phosphoric Acid Fuel Cell (PAFC), Molten Carbonate Fuel Cell (MCFC) and Solid Oxide Fuel Cell (SOFC) technologies were developed in the past decade. Each type of fuel cells has their own characteristics and fits to different applications. SOFC can use naturally existed resources such as natural gas, synthesis gas (Syngas), diesel and even hydrogen sulfide ($H_2S$), which is a major impurity component of natural gas in North America, as the fuel. The catalyst of SOFC should be tolerant to poisoning from fuel impurities. SOFC works at intermediate temperature range, i.e. 600$-$800$^\circ$C, to maintain ionic conductivity of the electrolyte. This is a temperature at which exhaust heat can be recovered through turbine generators to get higher overall efficiency and is a temperature that is not too harsh to materials. These characteristics make SOFC the one that will most likely capture markets of million watts scale stationary power generation, kilo watts scale residential power and heat supply, as well as smaller scale for truck auxiliary power unit (APU) (Larminie and Dicks, 2003).

Research and development activities of SOFC have been very active in both academic community and the industry. Academic researchers mainly focus on fundamental theory, such as modeling, simulation, and investigation of catalysis and electrolyte property etc. while the industry developers mainly focus on developing prototypes. In United States, the department of Energy (DOE) initiated the Solid State Energy Conversion Alliance (SECA), which combines government, industry, and scientific community to promote the development of SOFC. Siemens Power Generation, GE Global Research, Cummins Power Generation and other major SOFC developers are all participants of this organization. In addition, UTC Power, Rolls-Royce etc. also participate in the development of SOFC systems.

With numerous R & D efforts, SOFC technology has now evolved to the pre-commercial stage. Current SOFC prototypes reach the milestones of operating over 3000 hours without significant voltage drop and the costs have been reduced to $700 per kilo watt. According to SECA, goals of 2010-2015 would be the scale-up of SOFC prototypes, aggregation, integration, and validation of SOFC systems, continually increase the durability, and develop failure analysis methods etc. (Surdoval, 2009).

With these new developments, attention on the operation and control problem is increasingly getting the momentum. Most efforts so far have focused on improving properties of SOFC materials, such as power density, catalysts activity, electrolyte conductivity etc. Operation and control of SOFC have not been a main consideration until recent years. To achieve the new objective, understanding of SOFC dynamics is the very first and necessary step. Due to various reasons, experimental study of the SOFC dynamics has been difficult and rare at this stage (Bhattacharyya et al., 2009). First principle modeling therefore becomes a dominant option. Unlike detailed static modeling, dynamic modeling is to study dynamic properties of SOFC. In addition to control applications, investigation of durability and failure analysis also need the understanding of the SOFC dynamics.

3. MAIN COMPONENTS AND GOVERNING TRANSPORT EQUATIONS

A typical fuel cell consists of an electrolyte in contact with anode and cathode on either side as shown in Fig.1. Hydrogen rich fuel and air are continuously fed into the fuel cell for generating electricity. The electrolyte acts as a barrier between anode and cathode allowing only certain types of ions to pass through it. In a planar SOFC, several cells are stacked and connected in series to complete the circuit. At each cell, hydrogen releases electrons at the anode surface which travel through the outer circuit and combine with oxygen to produce oxide ions. Electrolyte which acts as a separator between hydrogen and oxygen, and thus prevents direct combustion. SOFC usually uses $Y_2O_3$-stabilized $ZO_2$ (YSZ) as electrolyte which allows oxide ion to pass through it to reach the anode surface, where the oxide ion combines with H+ to form water.

From perspective of transport, a fuel cell consists of several components: flow channels (including fuel flow channel and air flow channel), electrodes (including anode and cathode), electrolyte, and interconnector. The fuel and air are fed into fuel flow channel and air flow channel, respectively. These flows gradually across the interfaces, perpendicular to the flow direction, between the flow channels (fuel and air channel respectively) and the electrodes (anode and cathode respectively), diffuse through the porous electrodes, and arrive at the interfaces between the electrodes and the electrolyte, where the electrochemical reaction occurs and current is generated. A great effort of dynamic modeling has been spent on the transport dynamics of the flow channels and electrodes. The details of the two core components and governing equations are therefore given below:

The flow channels The key function of flow channels is to allow the distribution of gases throughout the fuel cell to the porous electrodes with as little losses as possible (Vandersteen et al., Sept. 2004). The governing transport equations include:
The conservation of mass:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0
\]
where \(\rho\) is the density of the flow in the channels, \(\mathbf{v}\) is the velocity vector.

The conservation of momentum:
\[
\frac{\partial }{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{\tau}
\]
where \(p\) is the pressure in the channels and \(\mathbf{\tau}\) is the stress tensor.

The species balance equation:
\[
\frac{\partial }{\partial t}(\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i) = -\nabla \cdot \mathbf{J}_i + r_i
\]
where \(Y_i\) is the mass fraction of the ith species in the channels, \(\mathbf{J}_i\) is the diffusive flux of the ith species, and \(r_i\) is the rate of production of species \(i\) per unit volume.

Energy conservation:
\[
\rho C_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T + \dot{q}
\]
where \(C_p\) is the specific heat, \(T\) the temperature, \(k\) the thermal conductivity, and \(\dot{q}\) the heat source term per unit volume, in terms of substance in the flow channel.

In all the above transport equations, some additional terms such as the heat terms due to convection and radiation appear as boundary conditions (Bhattacharyya et al., 2009).

The electrodes The porous electrodes of fuel cells are where the electrochemical reaction takes place. These electrodes serve several functions: allow for gas transport/diffusion through the pores to the active sites, and provide a site for the electrochemical reactions to occur (Vandersteen et al., Sept. 2004). The governing transport equations include:

The species balance equation:
\[
\varepsilon \frac{\partial }{\partial t}(\rho Y_i) = -\nabla \cdot \mathbf{J}_i + r_i
\]
where \(\varepsilon\) is the porosity of the electrode, and \(r_i\) is the rate of production of species \(i\) per unit volume within the electrodes. Note only the diffusion is considered in the electrodes.

Energy conservation:
In the porous structure, the energy conservation can be written by ignoring the convective heat transfer.
\[
\rho C_p \frac{\partial T}{\partial t} = k \nabla^2 T + \dot{q}
\]
where \(\dot{q}\) includes the heat generated by the current flow through the electrodes (Ohmic losses) and the activation losses, and the heat due to chemical reactions.

Once again additional terms such as heat terms due to convection and radiation appear as boundary conditions.

4. DYNAMIC MODELING OF SOFC

This section starts from the source of energy generation, followed by various losses of the energy, and concluded by analyzing the dynamics that affect energy generation and the losses. The model validation problem and other related progress in modeling aspect will also be discussed at the end of the section.

4.1 Dynamic Modeling in Electrodes

Source of Energy In the interface between electrodes and electrolyte, electrochemical reaction occurs. SOFC converts chemical energy of fuel and oxidant to electrical energy through reactions (Larminie and Dicks, 2003):

anode: \(H_2 + O^{2-} \rightarrow H_2O + 2e^-\)
cathode: \(\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}\)

The reaction not only releases electrons, but also builds up difference of potential energy between anode and cathode. This difference is called electromotive force (EMF), or more often, open circuit voltage (OCV). The OCV has been well studied, both theoretically and experimentally. It is affected by partial pressures and temperature, modeled by the Nernst equation (Larminie and Dicks, 2003):
\[
E = E^0 + \frac{RT}{2F} \ln \left( \frac{p_{H_2}p_{O_2}^\beta}{p_{H_2O}} \right)
\]

When anode and cathode are connected through an external circuit, the released electrons flow from anode to cathode and thus sustain continuous reactions. The electron flow is called current. The current produced is therefore related to the fuel consumption rate (Larminie and Dicks, 2003):
\[
i = 2FJ_{H_2} = 2FJ_{H_2O} = 4FJ_{O_2}
\]

Once the external circuit is closed, the voltage of fuel cell drops because of losses including activation losses, ohmic losses, and concentration losses, elaborated below.

Activation Losses Like all other chemical reactions, electrochemical reaction must overcome energy barriers for the reaction to proceed. This leads to activation losses, which is mainly due to the charge-transfer resistance between the electrodes and the electrolyte. Activation losses are usually described by the Butler-Volmer equation (Chan et al., 2001):
\[
i = i_0 \left\{ \exp \left( \beta \frac{nF\eta_{act}}{RT} \right) - \exp \left[ - (1 - \beta) \frac{nF\eta_{act}}{RT} \right] \right\}
\]

If only static response is considered, the operational voltage of fuel cell can also be modeled by (Larminie and Dicks, 2003):
\[
V = E - iR_m - A \ln \left( \frac{i}{i_0} \right) - B \ln \left( 1 - \frac{i}{i_l} \right)
\]

Concentration Losses The electrical chemical reaction occurs at the interface between the electrode and the electrolyte, called triple phase boundary (tpb). Fuel gas must pass through the porous electrode to reach the reaction site. The transportation in porous media is mainly through diffusion, and it is driven by concentration gradient. Therefore the actual fuel concentration and flux at reaction site is lower than that in the fuel channel. This is called concentration losses. Namely, the partial pressure of the reactant on the reaction site is lower than that in the supply of
the reactant. This phenomenon affects both static and dynamic properties of fuel cells. Due to the mass transfer dynamics, if there is a sudden increased demand in the current, it will take time to build a concentration gradient to produce required partial pressure on the reaction site. That is why the operational voltage drops significantly immediately after a higher current demand. Therefore, the transport process along the flow channels and along the electrodes limits the load following ability of the fuel cells.

Padullés et al. (2000) creatively interpreted the physical processes of SOFC through a block diagram, from the perspective of control. Their work clearly shows how current and fuel supply affects partial pressures on $tpb$ and therefore affects the voltage. They assumed SOFC stack as a choked, isothermal, lumped parameter system. By means of mass conservation, they modeled reactant partial pressures dynamically and applied them to the Nernst equation. Current is treat as a dynamic model input, which is proportional to the reactant consumption rate and therefore affects the partial pressures. The species dynamic model of Padullés et al. (2000) becomes the foundation of many other lumped dynamic modeling studies (Zhu and Tomsonic, 2002; Sedghisigarchi and Felachi, 2004).

Qi et al. (2005) adopted Fick's Law to describe diffusion along the porous electrodes. The mass transfer process along the anode is described as a partial differential equation with respect to time and space. By means of a Laplace transformation, the dynamic mass transport equation is converted to dynamic correlations between concentration at the reaction site and that at the fuel channel, in the form of transfer functions.

Diffusion can also be modeled by Stefan-Maxwell (SM) formula or Dusty Gas Model (DGM). Some researchers have compared the accuracy and found DCM is more accurate than SM and Fick's law (Bhattacharyya et al., 2009).

**Ohmic Losses** The internal resistance also reduces the operational voltage. Qi et al. (2005) modeled the ohmic losses dynamically by considering the effect of double layer capacitance and inherent resistance. The effect was simulated by an equivalent RC circuit which is an alternative of the equivalent circuit proposed in Larminie and Dicks (2003). The dynamics of the equivalent circuit was then modeled by ordinary differential equations (ODE).

In addition to the losses as discussed, there are also transport losses in the flow channels, i.e., the losses by the gas transport from the entry of flow channels to the interface between the flow channel and the electrodes. This is discussed in the next section.

### 4.2 Dynamic Modeling in Flow Channels

To maintain the electrochemical reaction, fuel and oxidant, must be delivered to reaction sites. Reactants are supplied through the flow channels. Mass transport determines fuel concentrations in the channel. For Syngas fuel, the transport in the fuel flow channel gets more complex with reforming/shifting reaction. The flow in the channels can be described by the mass conservation and the momentum conservation, as described by Equations 1-3.

Xue et al. (2005), Campanari and Iora (2004), Gemmen and Johnson (2005), Iora et al. (2005), and Jiang et al. (2006) modeled the fluid dynamics of fuel flows. Following similar modeling approaches, Cheddie and Munroe (2007), Kopasakis et al. (2008), and Xie and Xue (2009) investigated distributed voltage due to the fuel flow dynamics.

More practically, the fuel of SOFC is Syngas, which is a mixture of $\text{CH}_4$, $\text{H}_2$, $\text{CO}$, $\text{H}_2\text{O}$, and $\text{CO}_2$. While $\text{H}_2$ and $\text{CO}$ can directly participate in the fuel cell electrochemical reaction, $\text{CH}_4$ and $\text{H}_2\text{O}$ can generate $\text{H}_2$ and $\text{CO}$ through reforming/shifting reaction with cataclytical aid in anode:

\[
\text{Reforming: } \quad \text{CH}_4 + \text{H}_2\text{O} = 3\text{H}_2 + \text{CO} \\
\text{Shift: } \quad \text{CO} + \text{H}_2\text{O} = \text{H}_2 + \text{CO}_2 \tag{11}
\]

In addition to axial flow transport, $\text{H}_2$ and $\text{CO}$ in the fuel flow channel diffuse into anode and the reaction products in the anode such as $\text{H}_2\text{O}$ and $\text{CO}_2$ diffuse back to the fuel flow channel. The swap actually changes density of the fuel flow and therefore the momentum. So the velocity along the axial direction of the flow channel is no longer constant. The reforming reaction is endothermic, and it occurs on the surface of anode, with the aid of anode catalyst and heat from the cell. The shifting reaction occurs in the main flow body. It is slightly exothermic and therefore also heats up the fuel temperature (Qi et al., 2006a).

By considering the reacting fuel flow, Qi et al. (2006a) modeled detailed dynamics of SOFC through a finite volume approach, combining mass transport in porous anode, energy transport between solid cell and gas phase fuel, heat transfer between solid cell and fuel, and fluid dynamics of the reacting fuel flow in fuel channel. The model was presented as state space equations and the dynamics were studied through simulations.

Recent publications of Kang et al. (2009), Hajimolana and Sorounsh (2009) and Xi and Sun (2009) also combined the effect of reforming/shifting reactions in dynamic modeling. They studied the distributions of each species in the fuel channel and dynamic responses for major variables. Noticeably, Xi and Sun (2009) performed frequency domain analysis through their dynamic model.

Other than the losses that have been discussed so far, the governing equation for the energy generation and losses mechanisms are all related to temperature dynamics. Thus it is critical to model the temperature dynamics correctly through energy conservation.

### 4.3 Modeling of Temperature Dynamics

As we noticed in the Nernst equation, temperature has a direct effect on the voltage. Thus it is necessary to model the temperature dynamics. Dynamics of the SOFC temperature are governed by energy conservation law as described by Equations 4 and 5.

The overall SOFC cell can be seen as an exothermic device, because the current consumed by the internal resistance converts to heat and the electrochemical reaction itself is exothermic reaction. So the temperature of SOFC cell is usually higher than its environment. Unless it is well insulated, the heat exchange between fuel cells and its surrounding environment should also be considered. Inside
SOFC, conduction, convection, and radiation may all exist and heat exchanges strongly depend on the geometry.

Achenbach (1994) modeled the temperature of a planar SOFC stack in three dimensions. The purpose was to study temperature distribution of a planar SOFC. In addition to the heat produced by the SOFC cell, the model considered convection heat exchange between the cell and the fuel gas. Ota et al. (2003) modeled the temperature dynamics of a tubular SOFC in one dimension, and conduction, convection and radiation were all considered. Not only were the temperature distributions modeled, the dynamics of temperature was also investigated through simulation. Qi et al. (2006a) modeled the temperature dynamics on a finite volume of a tubular SOFC. The main purpose was to study the mechanism that is behind the temperature dynamics. Reaction heat, heat produced from the internal resistance, conduction, convection, radiation, and the dynamics of heat exchange due to gas flow velocity and due to fuel reforming/shifting reaction etc. were all considered in their modeling work (Qi et al., 2006a).

Ota et al. (2003) and Qi et al. (2006a) adopted the concept of enthalpy to model reaction heat. The use of enthalpy is convenient and naturally associated with energy carried by mass flow. Considering interactions of temperatures among the cell, fuel, air, and other solid parts of the SOFC stack, Qi et al. (2006a) also modeled the temperature dynamics of fuel flow, air flow and other solid components. The study of the fuel temperature dynamics is especially important, because it directly affects the reforming/shifting reaction and therefore performance of the entire stack.

Heat transfer through radiation should not be neglected since SOFC operates at high temperature. Several researchers (Xue et al., 2005; Iora et al., 2005; Qi et al., 2006a) considered the radiation heat transfer between solid components. However, most researchers neglected the radiation heat absorbed by fuel and air flow. Since the fuel flow contains high portion of methane CH4, steam H2O, and CO, the radiation heat that is absorbed by the fuel flow should be considered (VanderSteen and Pharoah, 2006).

Besides detailed models, Sedghisigarchi and Feliachi (2004) combined heat transfer dynamics of Achenbach (1994) and species dynamics of Padullés et al. (2000) to form a new lumped model, and simulated the lumped dynamic responses. Hall and Colclaser (1999) also studied the temperature dynamics through a lumped model.

With numerous dynamic models available in the literature, developed mostly from the first principles, a natural question arises, which is how to validate them.

4.4 Challenges: Validation of Dynamic Models

Conducting experiments to test dynamic responses of SOFC is still considered to be difficult due to the difficulty in setting up the experiment, such as where to place thermocouple to measure the electrode temperature without interfering its dynamics. The repeatability of fuel cell dynamic performance is also a problem. Existing literatures about the dynamic experiment of SOFC are sparse. Therefore, most of the dynamic models developed have not been validated through experiment data (Bhattacharyya et al., 2009).

Although direct experiment validation is difficult, several researchers have attempted to validate models through other indirect methods. For example, by comparing the Nyquist plot of the model with the experimental Electrochemical Impedance Spectroscopy (EIS) tests, Qi et al. (2005) validates part of dynamic models they developed. By comparing the simulated steady state concentration losses at different external load with the experimental V-I curve of Tsai and Barnett (1997), Qi et al. (2005) also validated their diffusion dynamic model. However the comparison of the steady state simulation results with experiment V-I curve should not be overstated (Vandersteen et al., Sept. 2004). Because there are many parameters in SOFC models, many different combinations may produce same V-I curve (Vandersteen et al., Sept. 2004).

Another indirect validation approach is to compare simulated dynamic responses from various and independently developed models available in the literature, as Sedghisigarchi and Feliachi (2004) and Qi et al. (2006a) did. Although validating SOFC dynamic models as a whole is difficult, the model describing each single mechanism has been well studied and validated such as the model of OCV, conduction, convection, and diffusion. Gemmen and Johnson (2005) studied the dynamic response of voltage and current of a button cell to load step change through experiments. Their lumped dynamic model considering the cell temperature dynamics was validated by comparing the experimental voltage responses to load step change. Saarinen et al. (2007) and Ollikainen et al. (2007) studied the SOFC stack operated at VVT through experiment. The effect of reforming/shifting reaction was their focus. But unfortunately, only simulated dynamics were actually published.

The dynamic modeling and experimental validation conducted by Bhattacharyya et al. (2009) is a valuable step forward. Supported by NanoDynamics Inc., Bhattacharyya et al. (2009) conducted the step response test of voltage and current by changing the load and the fuel flow rate. The SOFC they have studied is a tubular one running under H2 and air.

4.5 Analysis and Discussions

To summarize, dynamics of SOFC are mainly originated from five sources. They are: dynamics due to the electrochemical reaction; dynamics due to diffusion within electrodes, dynamics due to internal impedance; dynamics due to mass transfer in fuel channels; dynamics due to heat transfer.

Electrochemical Dynamics Catalysts for the anode and cathode facilitate electrochemical reaction. The electrochemical reaction is fast and it is not a limiting step. The reaction rate is faster than the rate at which the reactants can be delivered to the tpb. So the dynamics due to the electrochemical reactions can practically be neglected.

Diffusion Dynamics Although diffusion is the major resistance to the fuel delivery in electrodes, however, the
path of diffusion (or the thickness of porous electrodes) is short. The dynamics led by diffusion is therefore not significant, in the time scale of milliseconds (Qi et al., 2005). This has been confirmed by the EIS test.

The practical effect of porous electrodes and the diffusion is that reactant concentrations at the tpb are lower than at flow channels. So the voltage is lower than what can be expected from the supplied reactants concentration in flow channels.

**Internal Impedance Dynamics** Due to the existence of internal Ohmic resistance in electrodes and interconnectors, ionic resistance of the electrolyte, and the double layer capacitance between electrodes and the electrolyte, the operational voltage of SOFC is reduced. The resistance and the capacitance form a RC circuit. Time scale of this dynamics is also in the range of milliseconds and overlapped with the dynamics of diffusion (Qi et al., 2005).

**Mass Transfer Dynamics** Dynamics led by mass transport in flow channels strongly depend on the stack geometry. For a choked stack, time scale of reactant concentration response in the stack could be in the scale of several seconds (Padullés et al., 2000). For a regular tubular design, the space time of the flow channel is less than one tenth of a second. The concentration response dynamics is therefore also in this time scale (Qi et al., 2006a, 2008; Bhattacharyya et al., 2009). In planner SOFC, for the purpose of higher fuel utilization rate, the flow rate is usually lower. So the dynamic scale is higher, usually in the range of seconds.

The shifting reaction is fast, almost instantly. The reforming reaction rate is in the similar order of flow velocity. Therefore the reforming reaction mainly affects species distributions along the flow direction (Qi et al., 2008).

**Temperature Dynamics** Due to relatively large heat capacitance and relatively large mass of solid phase SOFC cell and other solid phase components such as the air guidance tube, the cell temperature dynamics are in the time scale of hundreds of seconds. Depending on the geometry, the temperature dynamic constant can range from 5-10 seconds (Ota et al., 2003) to 500-1000 seconds (Hall and Colclaser, 1999). Usually, the tubular SOFC design of Siemens Power Generation has the temperature time constant of around 200 seconds (Sadghisigarchi and Feliachi, 2004; Iora et al., 2005; Aguiar et al., 2005; Qi et al., 2006b; Cheddie and Munroe, 2007; Qi et al., 2008; Bhattacharyya and Rengaswamy, 2009b). The temperature dynamics play the dominated role in SOFC dynamic responses. It affects almost dynamics of every other mechanisms.

**Summary of Dynamic Effects** Great efforts have been put on study of the load following property of SOFC. When the external load changes, the reaction rate at tpb changes immediately. The concentration at tpb therefore also changes immediately and the concentration gradient in the porous electrode is changed quickly in turn. The new concentration gradient drives reactant flowing along the electrode to reach the new balance. This process is in the time scale of milliseconds (Qi et al., 2005). Then the new rate breaks the balance of the fuel channel. Both mass transport and reforming/shifting reaction are affected and will reach a new balance. The time scale of this process is in the range of seconds (Qi et al., 2006a, 2008).

On the other hand, the current change also produces different heat by the internal resistance. The changed reaction rate also leads to different reaction heat flux. The balance of the cell temperature is therefore broken. It needs hundreds of seconds to reach the new balance (Hall and Colclaser, 1999; Ota et al., 2003; Sadghisigarchi and Feliachi, 2004; Iora et al., 2005; Aguira et al., 2005; Qi et al., 2006b; Cheddie and Munroe, 2007; Qi et al., 2008; Bhattacharyya and Rengaswamy, 2009b). This process affects the entire heat transfer and therefore dominates the dynamics of electrochemical reaction, reforming/shifting reaction, and reactant temperatures.

4.6 Other Development and Applications of Dynamic Models

First principle models are nonlinear models and usually complex. To simplify, some researchers adopted simple model structures and then estimated the coefficients from the simulation of first principle models. Some other researcher directly simplified the first principle models.

Jayasankar et al. (2009) studied identifiability and estimability of a dynamic state-space model. Bhattacharyya and Rengaswamy (2009a) identified the diffusion process with dynamic experiment. They also simplified models using black-box format such as ARX and NAARX, and then identified the model coefficients from the simulations of the first principle model plus some experiment date.


Unlike techniques that convert first principle models to other simple formats, Flemming and Adamy (2008) developed a dynamic model from the qualitative linguistic description of the input/output relations by using continuous-time recurrent fuzzy system.

To develop a simple 1-D dynamic model, Qi et al. (2008) proposed an approximate analytical solution to deal with the distributed dynamic reacting gas flow problem. By this
5. SOFC CONTROL

Development of process models and design of the controllers are part of the advanced process control strategies. They are intricately dependent on each other. For example, the form of the models, whether the first-principle model or data-based, linear or nonlinear, 0-D or 3-D model, affects the design of the controllers. Thus, modeling of a process should always be based on the objective. A simple control relevant model may perform better than a complex 3-D model, which on the other hand, may be suitable for design and performance analysis of the process. Similarly, controller design techniques should be object oriented. A process expressed by a very complex model may be controlled by a regular PID controller. On the other hand, a simple process may have a lot of environmental and economic constraints requiring multivariate controller to maintain the optimal performance of the system. The solid oxide fuel cell system exhibits highly nonlinear characteristics together with a number of operation constraints; thus it needs special attention in designing controllers.

Recent advances and growing interest in fuel cells have led to a lot of activities on the modeling of fuel cells and their components as discussed in previous sections. Most of these models range from zero dimensional to complex three-dimensional models and also cover the area of performance evaluation and optimal design of the fuel cells. Some work has also been done on control relevant models that sufficiently describe the fuel cell system dynamics and yet are simple enough to build controllers ranging from simple PID to nonlinear model predictive controllers.

Therefore, in parallel to the modeling, some studies on the control of fuel cell systems have been published. Most of these papers dealt with load following performance of different types of fuel cells including polymer electrolyte membrane fuel cell (PEMFC), molten carbon fuel cell (MCFC) and solid oxide fuel cell (SOFC) by employing localized or, multi-loop controllers. Fewer papers considered controlling the entire fuel cell system by utilizing the constraints handling power of model predictive control. Only a handful of papers focused on control of solid oxide fuel cells.

5.1 Control Objective

As shown in Figure 2, a fuel cell system includes many components in addition to the fuel cell itself. The components are built around the fuel cell to maximize the efficiency of the system which, depending on the objective, may include additional heat exchangers, turbine, boiler, DC-AC converter etc. Optimal operation of the system thus requires efficient operation of these integral components, which put constraints on the overall operation of the fuel cell system. Designing a controller for a fuel cell system...
has to address the following issues: i) handle the abrupt change nature of the fuel cell voltage during transient operation, ii) reach the target load efficiently, iii) meet the constraints set by the different components safe operation limit, and vi) improve efficiency.

The first two issues, which are accompanied by a sudden instantaneous change of voltage for a change in the load, may be handled by designing simple load following controller such as PID by changing fuel flow (Zhu and Tomsovic, 2002; Chaisanthikulwat et al., 2008). The performance of the controller can be improved with the addition of a capacitor to filter the effect of sudden change of load and provide enough time for the employed controller to act on disturbance rejection (Murshed et al., 2010; Payman et al., 2008; Auld et al., 2008). It can be easily shown that any change in the load is accompanied by an instantaneous change in the stack voltage. The change in the stack voltage cannot be avoided no matter what type of advanced control is used due to the limit on the fuel and air flow rates. To avoid this sudden loss in voltage and possible damage to electrical equipment, an ultra-capacitor of sufficient capacity can be used in parallel with the fuel cell as an auxiliary power source. The advantage of the capacitor can be seen intuitively when there is a sudden change in the demand current, the capacitor will share the load and provide additional power. Thus, instead of sudden drop in the stack voltage, it drops smoothly depending on the capacitance of the ultra-capacitor. This gives an added boost to the controller connected to the SOFC system to keep the voltage at its referenced value. By avoiding sudden drop of the voltage the controller copes with only the slow change of the voltage and can bring the voltage at its reference value by increasing fuel flow rates within its constraints more easily.

The main constraints of any equipment stem from its design capacity. Thus for a solid oxide fuel cell, while the primary objective is to deliver the desired power at optimal efficiency, it is important to operate the fuel cell within certain limits. Since the operating temperature of SOFC is relatively higher than other fuel cells, the thermal stress among different components due to different temperature distribution along the anode, cathode and electrolyte can be detrimental for the integrity of the entire fuel cell. Thus it is of utmost importance to keep the maximum cell temperature below a certain threshold as well as reduce the temperature gradient. In addition, the partial pressure differential between fuel and air within anode and cathode, respectively, can also be of concern and should be kept below a certain value as per the design. Aside from the physical constraints of the fuel cell itself, limits on fuel utilization, fuel and air flow rate and constraints stemming from design of balance of plants play role in the operation of the fuel cell. For example, the lower limit imposed on the steam to carbon ratio at the entrance of the pre-reformer to avoid carbon deposition can be a limiting factor in the operation of the fuel cell (Aguiar et al., 2005). A sample list of operating limits of tubular solid oxide fuel cell is provided in Table 1 for illustration.

A sample control target for the operation of a fuel cell system could be defined as follows: i) maintain the stack voltage at its reference value by increasing fuel flow rates, ii) reach the target load efficiently, iii) meet the constraints set by the different components safe operation limit, and vi) improve efficiency.

### Table 1. Constrains summary of a tubular SOFC from section 7.2.1 of Fuel Cell Handbook, Edition 7:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Typical range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1 - 10 atm</td>
</tr>
<tr>
<td>Temperature</td>
<td>650 - 1050 °C</td>
</tr>
<tr>
<td>Partial pressure of oxidant</td>
<td>0.16 - 0.20</td>
</tr>
<tr>
<td>Ratio of partial pressure of fuel, $p_{H_2}/p_{H_2O}$</td>
<td>0.9 - 6.9 at 1000 °C</td>
</tr>
<tr>
<td>Current density</td>
<td>50 - 400 mA/cm²</td>
</tr>
</tbody>
</table>

---

**Fig. 2. Overview of a SOFC system**

required power output to its desired level, 2) keep the maximum cell temperature below the upper bound, 3) keep the fuel utilization within optimal operating limits for all power outputs. The fuel and air flow rates can be varied to achieve the above mentioned targets (Roberts et al., 2006; Stiller et al., 2006; Li et al., 2005) and thus act as manipulated variables (MV). In addition, depending on the objective, current density can be defined as either a manipulated variable or, a disturbance variable (DV) and so are the inlet temperatures of fuel and air. For univariate control scenario, power can be controlled by using fuel rate as an MV whereas flow rate of air can be used to control either the fuel utilization or, cell temperature. If fuel utilization is being controlled by moving the flow rate of air, an override temperature control can be used to keep the cell temperature below its maximum limit. In such case, the override temperature control will start to move the flow rate of air only if cell temperature exceeds its higher limit. Addition of a pre-heat exchanger, on the other hand, can provide an additional degree of freedom which can be utilized to maintain the cell temperature (Kaneko et al., 2006; Murshed et al., 2010). Another override controller can also be designed to keep the differential pressure between anode and cathode below its design capacity. Both the flow rates of fuel and air can act as MVs for the differential pressure override controller.

### 5.2 Applications of Various Control Techniques in SOFC

In the process control world, a wide range of linear and nonlinear control techniques have been developed and implemented in industries. Various controllers including traditional PID controllers, model predictive controllers,
and nonlinear model predictive controller (NMPC), have also been applied in the control of fuel cells.

For example, Zhu and Tomsovic (2002) have studied the load following performance of fuel cells and micro-turbine connected in a power grid. Ro and Rahman (2003) presented a method for dampening power oscillation of fuel cell devices connected in the electrical distribution network. El-Sarkh et al. (2004) designed a neural-network based controller for PEMFC, whereas Li et al. (2005) developed multi-loop control strategies for maintaining fuel utilization and voltage. Some papers discussed controlling electrical power of fuel cells connected in the power grid rather than considering the fuel cell system as a separate process. More recently several authors designed MPCs and fuzzy controllers for different types of fuel cell systems (Zhang et al., 2008). In the following, we will elaborate various control strategies, classified according to univariate and multivariate strategies.

**Univariate control**

For this class of control, the main objective is to generate constant power by maintaining constant fuel utilization and average temperature across the fuel cell. Often these targets can be achieved by careful design of single or multi-loop controllers based on the developed or, identified model. Most of these controllers are either employed through PID controller or as a ratio controller.

Kandepu et al. (2006) showed that the power, fuel utilization and cell temperature in a SOFC-GT system can be controlled by manipulating current, the fuel and air feed flow rates respectively, using PID control. In their work, several multi-loop controllers with rate limiter have been put in place to keep the fuel utilization and temperature within safe operating limit. It has been shown that the methodology works well at normal operating conditions but may show unstable temperature at lower load.

Stiller et al. (2006) analyzed the stable region of a SOFC-GT system and the objective of control. A multi-loop control strategy was developed to control the power output, fuel utilization, and the cell temperature. Kandepu et al. (2007) developed a lumped dynamic SOFC model and designed a similar control strategy as Aguilar et al. (2005) to verify the model quality for control. In order to control the SOFC system for rapid load following, a SOFC system configuration and a special control strategy were proposed in Mueller et al. (2007a) and some results were applied to a SOFC-GT system (Mueller et al., 2007b).

Chaisantikulwat et al. (2008) developed a 3-D dynamic model of an anode-supported planar SOFC. The model was derived from the partial differential equations representing the conservation laws of charges, mass, momentum and energy. A first order transfer function model was then obtained from the step response of the PDE model around nominal operating condition. The identified model, while is easy to obtain compared to first principal model, can be useful in designing multi-loop PID controllers or, multivariate controllers like MPC. However, if the operating condition significantly deviates from the nominal operating points, the simplified model would likely produce larger error. Similarly, Inui et al. (2006) used air utilization and inlet gas temperature of a planar SOFC to keep temperature distribution constant whereas Sorrentino et al. (2008) used a PI controller to regulate the SOFC temperature variation by manipulating the excess air flow rate. Kaneko et al. (2006), on the other hand, used a standard PID control strategy to manipulate fuel flow rate to maintain the power output of the system that accounts for the fluctuation of gas composition in the fuel. In addition to power control, fuel cell temperature is controlled by introduction and use of a bypass valve around the recuperator. By releasing excess heat to the exhaust, the bypass valve provided the control means to avoid the self-exciting behavior of system temperature and stabilized the temperature of SOFC.

The control objective of Hajimolana and Soroush (2009), on the other hand, is to maintain voltage and temperature by two decentralized PI controllers that use air flow and air inlet temperature as the control handles. Aguilar et al. (2005) managed to achieve temperature and power target by utilizing two control loops. The first loop is composed of a master controller that imposes a load change and sets the fuel and air flow rates proportional to that new current, keeping the fuel utilization and air ratio constant while the second loop responds to the temperature deviation by changing air ratio around the default value set by the master controller. It has been shown through simulation that, for moderate load changes, the PID temperature controller can successfully take the outlet fuel temperature to the desired setpoint. However, for higher load changes adjustable setpoint strategy was adopted to avoid oscillatory control action.

**Multivariate control**

As stated earlier, some constraints need to be satisfied due to physical and operating limits of the fuel cells in addition to meeting target power and temperature of the fuel cell. Even though simple single and multi-loop PID controllers often suffice in achieving the objective at nominal operating conditions, they cannot handle limiting constraints and are prone to failure under such scenarios. In addition, being highly nonlinear in nature, the model nonlinearities and constraints need to be taken into consideration while designing the controller. Nonlinear model predictive control which is an extension of well established linear model predictive control can be designed for this kind of applications.

A number of different well established nonlinear control methods are available in the literature ranging from generalized nonlinear model predictive control to the back-stepping method. Out of these nonlinear controllers, the reason that nonlinear MPC stands out with more advantage than other nonlinear controllers such as, the back-stepping method, comes from the complexity involved in designing these types of controllers. Development of nonlinear control like the back-stepping method is relatively simple when the model is of simple nonlinear nature and if the energy function is also available. For a complex nonlinear model, like the fuel cell and its system, it is not easy to derive an energy function that can lead to physically understandable and implementable control law. Even if the energy function is available, the deduction of the control law is difficult and, most importantly, it will not be able to handle the constraints. Thus more focus
has been put on designing linear and nonlinear model predictive control than any other types of control in SOFC.

**MPC in SOFC** Several authors have recently focused their attention on applying MPC on SOFC (Zhang et al., 2008; Jurado and Ortega, 2006; Yang et al., 2009; Wang et al., 2007; Huo et al., 2008b; Wu et al., 2008b). Zhang et al. (2008), in their work, developed a closed-loop feedback control strategy based on the NMPC controller for a planar SOFC. The main control objective was to control the output power, fuel utilization and temperature by manipulating the current, fuel and air flow rates. The authors used a moving horizon state estimator to predict mole fraction and temperature of the exit gases.

Using the idea of predictive control, Zhang and Feng (2009) proposed a fuzzy predictive tracking controller to achieve fast load following. Yang et al. (2009) proposed a predictive controller based on a T-S fuzzy model to maintain the stack temperature. Vijay et al. (2009) proposed a predictive controller based on the bond graph SOFC model that they developed. The load-following objective is achieved by manipulating air and fuel inlet and outlet valves. A secondary loop was adopted to control the cell temperature.

Wang et al. (2007) developed subspace based data-driven predictive control of SOFC. In this approach, the controlled variables were stack voltage, fuel utilization, ratio of partial pressure of hydrogen and oxygen, and fuel cell pressure difference between anode and cathode, of which only the voltage is measured. The manipulated variables were molar flow rate of hydrogen and oxygen, whereas the current demand is considered as disturbance.

Instead of using first principal model, several authors used fuzzy model to build model predictive control of a SOFC system (Jurado and Ortega, 2006; Wu et al., 2008b). Jurado and Ortega (2006) identified a fuzzy Hammerstein model by using input-output data, whereas Yang et al. (2009) used a Takagi-Sugeno (TS) fuzzy model. Wu et al. (2008b), on the other hand, applied a nonlinear model predictive control method based on an improved radial basis function (RBF) neural network, and a genetic algorithm in order to control the voltage and guarantee fuel utilization within a safe range.

### 5.3 A Sample MPC-for-SOFC System

As discussed above, model predictive control appears to be a right choice for the control of SOFC systems. Model predictive control has presented itself as the most successful process control technology in the recent years. Nonlinear model predictive control, which is a generalized version of the well-established linear model predictive control, can handle process nonlinearities and constraints. Based on measured or, estimated states at current time, it predicts future states and required control actions such that a predefined objective function is optimized over a predefined horizon. It then applies the first of the calculated control actions, and proceeds to the next time step, and then repeats the entire procedure. Mathematically the MPC formulation can be written as finding a set of future control actions \( u(k|k), u(k+1|k), \ldots, u(k+M-1|k) \) by solving the following optimization problem,

\[
\begin{align*}
\min_{u(k|k), u(k+1|k), \ldots, u(k+M-1|k)} J &= \sum_{i=1}^{N} \left( \| x(k+i|k) - x_{ref} \|_Q^2 \right) \\
&\text{subject to,} \\
\hat{x}(k+1) &= f(\hat{x}(k), u(k), w(k)) \\
x_{min} &\leq \hat{x} \leq x_{max} \\
u_{min} &\leq u_{k+i|k} \leq u_{max} \\
\Delta u_{min} &\leq \Delta u_{k+i|k} \leq \Delta u_{max}
\end{align*}
\]

where, \( N \) is the prediction horizon over which future states are calculated and the objective function is minimized; \( M \) is the control horizon over which control actions are optimized.

Consider a SOFC system as shown in Figure 2, methane is pressurized and fed to the fuel heat exchanger for preheating by the exhaust gas from the burner. The preheated methane then enters an external reformer along with steam where methane is converted to hydrogen through reforming and watergas shift reaction. The product gas from reformer enters into the anode compartment of the fuel cell stack. Pressurized air is also preheated in another heat exchanger by the hot exit gas from the fuel heat exchanger and sent to the cathode compartment of the fuel cell stack. Hydrogen from the anode compartment and oxygen from the cathode takes part into the electrochemical reactions to produce power at the electrode. The depleted fuel and air from the fuel cell stack is then fed into a burner to produce heat from the unreacted methane, hydrogen and carbon monoxide. The exhaust from the burner is then sent to the fuel and air heat exchanger consecutively as described earlier. The exhaust gas from the air heat exchanger is then sent for heat recovery in the form of steam and hot water.

Murshed et al. (2010) designed linear and nonlinear MPCs for this SOFC system, based on the above MPC formulation. In designing MPC for the solid oxide fuel cell system, fuel, steam and air flow rates are identified as the manipulated variables \( (u) \) which are calculated at every step to keep the main control variables, voltage and fuel utilization, on its target \( (x_{ref}) \). Depending on the objective and the availability of independent variables, the cell temperature, fuel utilization and differential pressure between the anode and cathode can be defined as control variables or, as constraints. Additional balance of plant components such as heat exchanger, splitter and burner can also provide additional degrees of freedom which can be used as manipulated variables. The demand current, the fuel and air temperatures are considered as disturbances.

Murshed et al. (2010) studied load regulation capability of both linear and nonlinear MPCs applied to the fuel cell system along with a capacitor connected in parallel with the fuel cell. In the design, the discretization of the nonlinear continuous-time model is performed by the orthogonal collocation method and the unmeasured states are estimated by using the unscented Kalman filter. In all cases, NMPC outperformed linear MPC in terms of load disturbance rejection. On the other hand implementation of NMPC needed larger computational power and time, which is an inherent disadvantage of nonlinear MPC.
Fuel cells convert chemical energy of the fuel directly into the electrical energy and thus can have high efficiency. The unreacted fuel can then be burned to produce additional energy. The high temperature exhaust from the fuel cell system can be used to generate further electricity using a gas turbine or simply produce hot water and steam for home and industrial use. Even though the indirect energy provides a good part of the fuel cell system power, the main objective for a fuel cell system is to produce as much direct energy as possible. Thus, a steady state optimizer can also be designed to minimize energy in the effluent gas of the fuel cell system. The output of the optimizer can act as a steady state reference to the dynamic layer of the MPC.

5.4 Challenges in SOFC Control

Several important issues need to be considered during the study of both univariate and multivariate controller. Some of these issues are discussed below:

- **Decoupling:** The multi-loop controllers are usually tuned for a nominal operating condition and may start exhibiting unstable/oscillatory behavior under different operating conditions as well as under large disturbances. Also due to inter-dependencies among different operating variables, it may take longer time to stabilize the system. The effect of interactions among different operating variables can essentially be removed by designing decoupler. Even though multivariate controllers such as MPC can stabilize the system without the need of decoupler, during start-up and/or, during unavailability of the multivariate controller, the system can be difficult to control. Thus efforts on the design of decoupler for the fuel cell system can, in the long run, be beneficial for the safe operation of the system.

- **Initial Value:** Initial value is important for the optimization algorithm in NMPC. If the initial state is too far away from the optimal point, the solution becomes infeasible. Same is true for steady-state optimization. This problem is particularly severe in SOFC NMPC study, due to strong nonlinearity and possibly multiple steady state points of SOFC. Further research is needed to reduce the sensitivity to the initial values.

- **Linear vs. Nonlinear MPC:** Even though nonlinear MPC has superior performance over linear MPC, implementation of NMPC is not straightforward. First, it requires a nonlinear first-principles model, development and maintenance of which requires significant time and effort. Moreover, any significant change in the plant also requires update of the model which may become a continuous effort in the long run. Linear models, on the other hand, can be updated by performing simple plant test. In addition, depending on the complexity of the model, there is need for longer sampling interval to estimate unmeasured states using nonlinear state estimator and execution period of the controller, so the computational time of nonlinear MPC can be much higher compared to that of the linear MPC. In view of this, a multiple linear model approach could be considered for SOFC modeling and control.

- **Temperature Gradient Control:** There are two main bottlenecks to taking SOFC to commercial applications: load following ability and durability. Process control can play important roles to improve both as discussed in this paper. However, one outstanding problem that has not been addressed in this review is the control of temperature gradient, which has a direct impact on durability. This is due to, in part, lack of suitable distributed dynamic models. The control-relevant distributed dynamic model developed by Qi et al. (2008) is relatively simple and can be useful towards this direction.

- **Monitoring:** A real-time monitoring system can safeguard fuel cell operations and is one of the focus of the current effort in SOFC development. Dynamic modeling, control and monitoring are the essential ingredients of fuel cell developments. However, the results on the real-time monitoring from the perspective of dynamics and control are relatively sparse and call for more research effort.

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sensitivity to the change of cell component thickness. Journal of Power Sources, 93, 130–140.


