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Dynamic Modeling of Solid Oxide Fuel Cell Systems for Commercial Building Applications

Andrew Schmidt and Robert Braun
Department of Mechanical Engineering
College of Engineering and Computational Sciences
Colorado School of Mines
1610 Illinois Street
80401 Golden CO USA
Tel.: +001-303-273-3650
Fax: +001-303-273-3620
rbraun@mines.edu

Abstract

A dynamic SOFC system model has been developed for the purposes of performing an engineering feasibility analysis on recommended integrated system operating strategies for building applications. Included in the system model are a dynamic SOFC stack, dynamic steam pre-reformer and other balance-of-plant components, such as heat exchangers, compressors and a tail gas combustor. Model results show suitably fast electric power dynamics (12.8 min for 0.5 to 0.6 [A/cm^2] step; 16.7 min for 0.5 to 0.4 [A/cm^2] step) due to the fast mass transport and electrochemical dynamics within the SOFC stack. The thermal dynamics are slower (17.4 min for 0.5 to 0.6 [A/cm^2] step; 25.0 min for 0.5 to 0.4 [A/cm^2] step) due to the thermal coupling and thermal capacitance of the system. However, these transient results are shown to be greatly dependent upon SOFC system operating conditions as evidenced by settling times of greater than 2 hours for a 0.3 to 0.24 [A/cm^2] step. In addition, system design implications on system dynamic response are revealed with particular attention on the effect of an external pre-reformer and the configuration of the process gas heat exchanger. Preliminary results are summarized within the context building load profiles and demand requirements.

Introduction

Integrating emerging distributed generation and renewable energy sources in a building has the potential to drastically improve the site's environmental impact, energy cost, and energy efficiency. With impending energy and environmental challenges, the successful application of these technologies is becoming increasingly important. There have been many technological and cost advances in photovoltaics, solid oxide fuel cells (SOFC), small-scale wind turbines, advanced batteries and thermal storage, which may lend themselves towards a commercial building or building cluster application on a micro-grid.

Recent research into the optimal integration and dispatch of SOFC systems in commercial building applications has shown optimal system designs that include renewable sources, SOFC systems, and thermal and electrical storage [1, 2]. These studies have also shown that in order to be cost-effective, some dynamic operation of the SOFC system in the form of load-following may be required (as opposed to a purely base-load operating strategy). Figure details example results of a commercial building-DG system design study for a large hotel in San Francisco, California. This system design and operation results in a 30% decrease in life-cycle costs over a grid-only case while utilizing anticipated near-term capital costs for the hardware [2]. The figure shows electrical load-following operation of the SOFC system throughout the day when on-site photovoltaic and wind turbine generation is present. Also evident in the figure is the large decrease in grid electricity purchase of the building. This decrease in grid electricity purchase lowers operating costs and results in net life cycle cost savings. However, the dynamic capabilities of entire SOFC systems are, as of yet, relatively unexplored computationally or experimentally and it is yet to be seen whether desired cost optimal system operation is feasible.

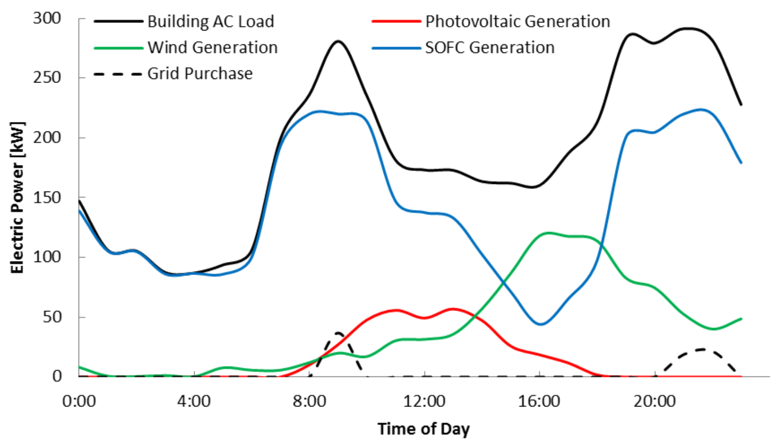

Figure 1: Example cost saving DG system operation for a large hotel in San Francisco.

The primary objective of this research is to develop dynamic modelling tools that enable the transient simulation of SOFC systems. This preliminary effort aims to evaluate the dynamic response of an SOFC system and identify noteworthy dynamic component interactions which system control schemes must address. Due to the mass of the SOFC stack and reformer, the coupling between stack inlet and outlet conditions from process gas heat exchange, and the restricted operating window for safe operation of SOFC stacks, the thermal and electrical dynamic response is expected longer than for SOFC stacks alone. Detailed investigation into the intra-system coupling is performed to examine the dynamic capabilities of an SOFC system intended for commercial building integration.

1. Scientific Approach

Figure shows the system design employed in the present study. The system component models include a tail gas combustor TGC, recuperative heat exchangers, reactant gas compressors, fuel cell stack and external steam reformer. Anode gas recycle (AGR) is included in the system design in order to provide steam for the pre-reformer and reduce axial thermal gradients within the fuel cell stack [3, 4].

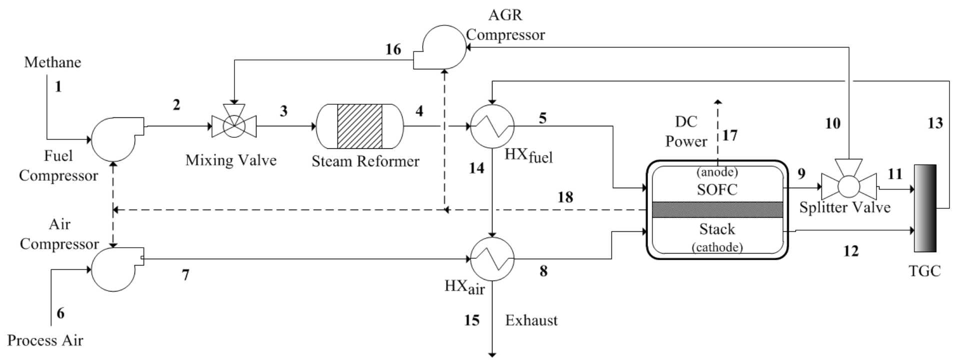

Figure 2: SOFC system flow diagram.

A dynamic SOFC stack model was developed for a one-dimensional, co-flow, internal reforming configuration [5]. Within the model, dynamic mass and energy balances are developed around spatially discretized control volumes. In addition, a momentum balance is approximated using a relationship between flow rate and pressure drop [6]. Activation, concentration and ohmic overpotentials are considered in the electrochemical sub-model. The model employs a linear extrapolation of single-cell performance to predict stack-level performance. The SOFC stack model integrity was established by benchmarking it with other stack models given in the literature [7, 8] and a maximum error of 2% was observed. Inputs to the stack model are fuel and air channel inlet flow rates, composition, temperature and pressure as well as the current load of the stack. The stack model outputs are fuel and air channel outlet flow rates, composition, temperature and pressure as well as stack voltage and power and spatial distribution of gas and solid temperatures, gas composition, and gas pressure.

The pre-reformer is modelled as an adiabatic, packed bed reactor constructed from a stainless steel cylinder filled with steam reforming catalyst. The steam pre-reformer model is adapted from the work of Murshed et al. [9]. This model is thermally lumped, employs a reforming reaction rate expression, and is dynamic in temperature only. It is assumed that the reformate gas exits the reformer at the reformer solid temperature. Included in the model are chemical reactions for steam reforming (SR) and water-gas shift (WGS).

All other system component models are steady state and have adiabatic boundary conditions with the surroundings. The TGC is modelled as a mixer that combusts the depleted anode fuel gas in a manner tantamount to making an adiabatic flame temperature calculation. Heat exchanger models assume constant effectiveness. Pumps utilize desired outlet pressure and isentropic efficiency to calculate the outlet conditions.

System model inputs are gas inlet temperatures, pressures and flow rates at statepoints (1) and (6) of Fig.2, as well as the total current load of the SOFC stack and the pressure at (2), (16) and (7). It is assumed that the SOFC stack can instantaneously meet the current load requirements and that the pumps change flow rates instantaneously.

2. Simulations

The component with the largest impact on dynamic response of the SOFC system is the ceramic stack due to its relatively large thermal mass. Thus, stack dynamics are analyzed first, in terms of gas outlet temperature and power output. This is followed by a similar analysis of the system dynamics.

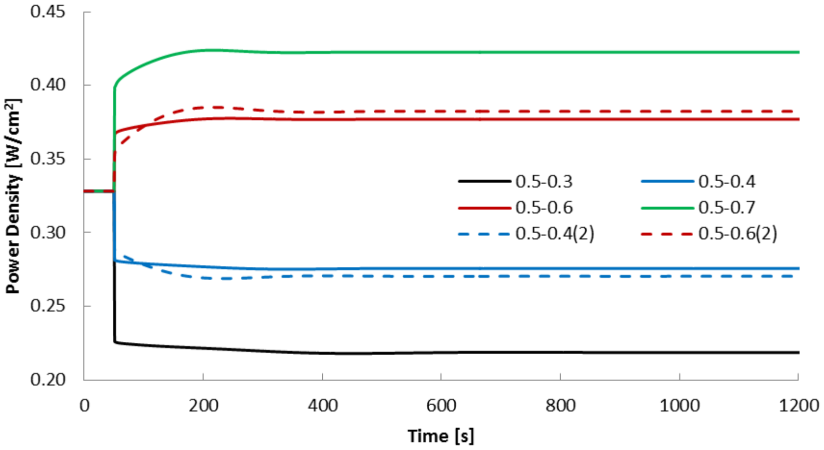

Figure 28: Dynamic power density at various current density steps with initial conditions of steady state at 0.5 [A/cm^2].

Figure 28 describes the cell power density as a function of time according to various current density steps. Two dynamic simulation cases are studied. In the first case, constant fuel utilization and air stoichiometric ratio are maintained throughout a change in operating current density (shown as solid lines in Figure 3 and designated as “strategy A”). Strategy A, assumes an instantaneous gas flow rate response in order to maintain constant utilization. In contrast, “strategy B” keeps the feed gas flow rates constant and allows the fuel utilization and stoichiometric ratio to vary as current density is altered. All cases initiate at steady state with a current density of 0.5 [A/cm^2], fuel utilization of 75% and air stoichiometric ratio of 8.5. Inlet conditions are 1023 [K], 1 [bar] and the fuel composition is a methane-steam gas mixture with a molar steam-to-carbon ratio of 2 that is pre-reformed 10% and in water-gas shift equilibrium.

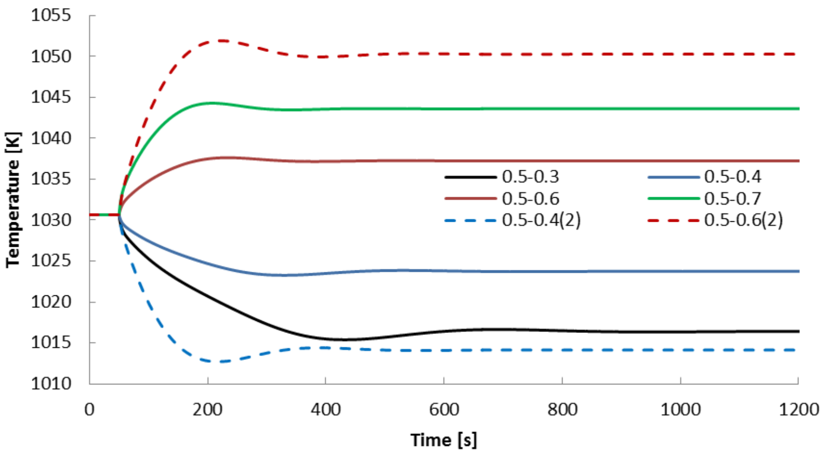

Figure 4: Dynamic average PEN temperature at various current density steps with initial conditions of steady state at 0.5 [A/cm^2].

As illustrated in Figure 3, the dynamic response of electric power production closely follows the trend of the current steps under which it was produced. There is an instantaneous change in power density which translates to the instantaneous change in voltage according to the inclusion of current density in the electrochemical overpotentials. For the 0.7 [A/cm^2] case, the ±1% settling time of power density (henceforth referred to as power settling time) is 201 [s] while for the 0.3 [A/cm^2] case, the ±1% settling time is 243 [s]. This settling in power output means that, relatively consistently, within about 4 or 5 minutes, the SOFC can change power output level to meet the building load.

Figure shows the dynamic response of the average PEN temperature of the SOFC stack with the same load steps as the previous analysis. It is evident that the dynamics of the cell are much faster at higher current densities, or lower efficiencies. Quantitatively, the ±1% settling time of the average PEN temperature (i.e., thermal settling time) for the step up to 0.7 [A/cm^2] case is 299 [s], compared to 724 [s] for the step down to 0.3 [A/cm^2] case. That is, a 142% difference in settling time between these cases is observed and is particularly relevant when considering deploying an SOFC system to meet a building electric load. The thermal settling time of the 0.4 [A/cm^2] case with strategy A is 543 [s] compared to 391 [s] with strategy B. This reduction in settling time suggests that faster thermal dynamic response comes at the expense of lower fuel utilization and, therefore, lower efficiency. The final fuel utilization and stoichiometric ratio are 0.60 and 10.63, respectively. However, the difference in time is less pronounced for smaller step sizes (e.g., the 0.1 [A/cm^2] step to 0.6 [A/cm^2]) case where the thermal settling time for strategy A is 360 [s] compared to 391 [s] for strategy B. In this case, settling time is actually increased by maintaining constant flow rates. Final fuel utilization and stoichiometric ratio are 0.90 and 7.1, respectively. Therefore, as seen from these simulations, the direction and magnitude of current density change has a large impact on the stack dynamics. However, the similarity in settling time for the two constant flow rate cases suggest that the change in dynamic response at different current densities is due to the changing mass flow rates.

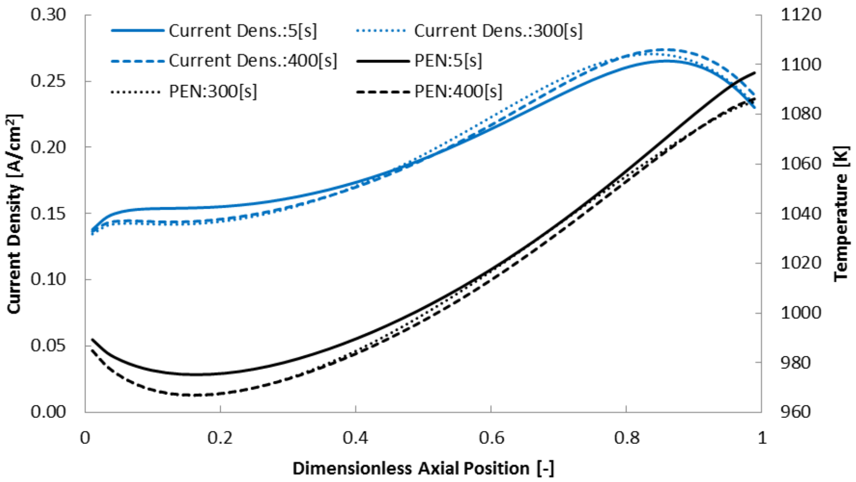

Figure 5: Current density and PEN temperature profiles at selected times.

The oscillations in the response are due to a complex interaction between current density and temperature distributions. Figure illustrates these effects and provides insight into the coupled phenomena. After the current load and inlet flow rates are instantaneously changed, the gas composition and material temperature states are not in steady state and the energy and mass balances force the states towards the steady state condition. For a current load decrease, this process results in a cooling effect on the PEN structure as there is less heat being released from the redox reaction even though there is also less electrical power produced. This cooling results in decreased operating voltage which reduces the electrical power output. As the cooling progresses at different rates across the cell, the current density and power output also change, but the average current density must stay constant resulting in a current density profile shift to maintain the constant current and a uniform cell voltage constraints. As the current density profile shifts, the cooling rate also changes: essentially, the operating voltage, and current density and temperature profiles are coupled non-linearly. Eventually, the current density and temperature profiles shift to the point where they overshoot the new steady state temperature distribution until the thermal inertia is damped by heat and mass transfer with the reactant gases. The thermal capacitance of both the gas streams and solids dampen and slowly diminish these oscillations. This dampening due to thermal mass explains the faster response at higher current densities (since larger flow rates are present).

Table 1: SOFC system parameters and operating conditions

Parameter	Value	Units	Parameter	Value	Units
Fuel utilization:	69%		Stoichiometric air ratio:	7.0	
Inlet fuel temperature:	26.85	C	Inlet air temperature:	26.85	C
Reformer reaction area:	2	m^2	Reformer volume:	0.0111	m^3
Reformer length:	0.25	m	Reformer case thickness:	1.5	mm
Fuel HX effectiveness:	0.6		Air HX effectiveness:	0.8	
Number of cells:	384		Operating SOFC pressure:	1.3	Atm
AGR percentage:	50%				

The cell dynamic analysis shows that SOFC stacks themselves have promising potential for commercial building applications as the electric power settling time is consistently faster than 6 minutes which is well within the hourly timestep of dynamic operation in current optimization studies. The analysis has also shown that maintaining constant flow rates throughout current transients generally increases settling time and does not improve the dynamic response. In addition, operation at lower efficiency improves the dynamic response of the stack due to the increased flow rates.

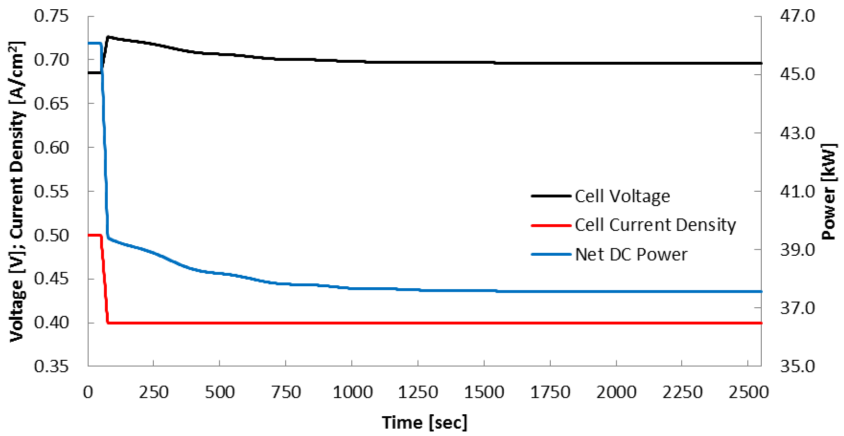

Figure 6: SOFC system electrical dynamics for ramp from 0.5 to 0.4 [A/cm^2].

A system dynamic simulation was performed after the dynamic characteristics of the SOFC were established. The following preliminary results have been calculated according to the operating conditions and system parameters presented in 1. Results are calculated using the noted current change over 50 [s] which closely simulates a current step when considering the long dynamic response of the system.

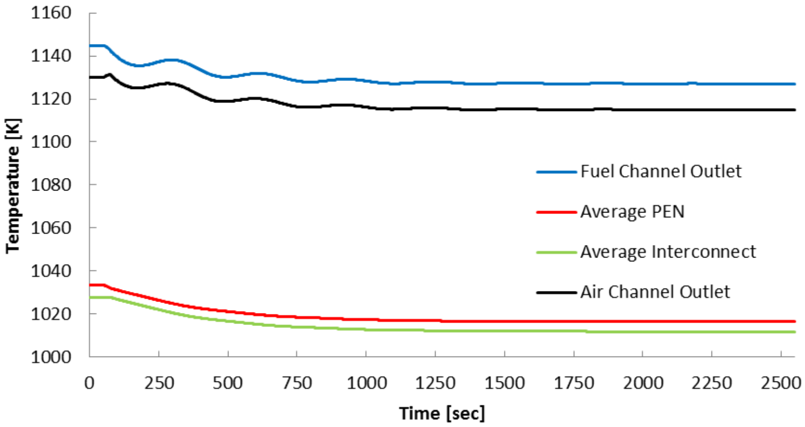

Figure 7: In-system SOFC stack thermal dynamics for ramp from 0.5 to 0.4 [A/cm^2].

Figure details the electrical dynamics of the SOFC system for a 50 second current ramp from 0.5 to 0.4 [A/cm^2] with constant fuel utilization and air stoichiometric ratio. The ±1% settling time for the net DC power output is 999 [s] or about 17 minutes compared to 3 minutes for the stand-alone SOFC stack. This 20% reduction in current load results in an 18.5% reduction in power output. The response dynamics are slightly oscillatory in nature, but of low amplitude; however this periodic result has implications for component coupling as discussed later. The voltage response initially increases, with the overpotentials instantaneously adjusting for the decreased current density. As the current density stops changing, the voltage then slowly decreases to its steady state value due to the decreasing PEN solid temperature as discussed below.

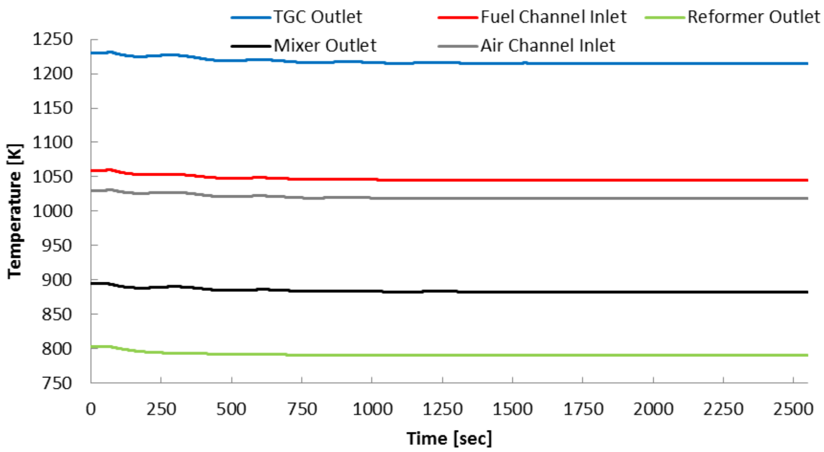

Figure 8: SOFC system temperature response for a fast ramp from 0.5 to 0.4 [A/cm^2].

Figure shows the thermal response of the in-system SOFC stack for this current load change. The average PEN temperature is slowly decreasing due to the decreasing amount of redox reaction occurring in the cell and increased efficiency. This lower conversion of chemical energy and the simultaneous increase in cell efficiency allows for the gas flows to carry heat out of the cell until the PEN solid reaches its steady state temperature. The average PEN temperature settles within 1% of its steady state value 1500 [s] after the load begins to change. Most noticeable in this figure are the more visible oscillations of the outlet gas temperatures. This occurs due to the inherent dynamics in the SOFC stack, especially during decreasing load changes. Recall that these dynamics occur due to the complex coupling between temperature and current density profiles. These dynamics are amplified compared to the stand-alone SOFC stack case due to the coupling of inlet and outlet stack gas temperatures from AGR and exhaust heat recuperation.

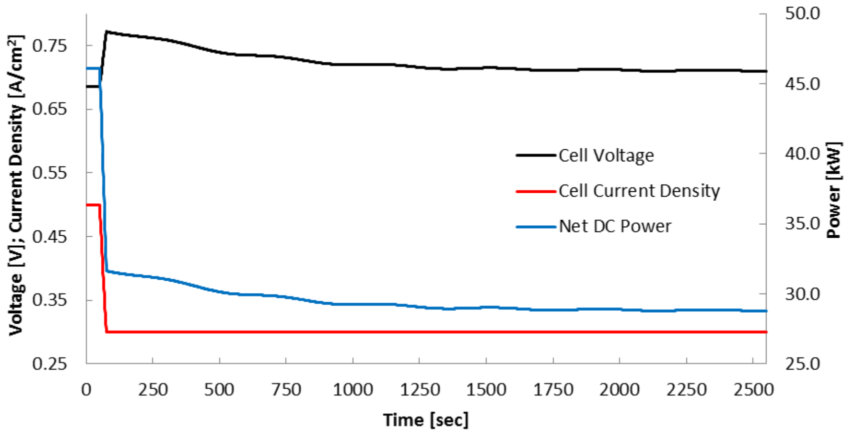

Figure 9: SOFC system electrical dynamics for ramp from 0.5 to 0.3 [A/cm²].

Figure details the temperatures of select state points in the system. The coupling between SOFC anode outlet and inlet is illustrated where the fuel channel inlet temperature is changing due to the AGR and recuperative heat exchangers. Since the reformer operates adiabatically, its thermal mass dampens out the fuel gas temperature dynamics thereby helping to manage the coupled oscillations at the stack. The reformer appears to have a relatively simple 1st order response with a ±1% settling time of 1322 [s]. The reformer response contains low amplitude oscillations due to the periodic inlet temperature, but the resolution of the figure does not permit these small oscillations to be visible. Although there is a transient response in the system components, the magnitude of these changes are small with the reformer temperature decreasing only 1.7% and TGC outlet temperature decreasing 1.2%. Compared to the stack-only response, the system thermal dynamics are about 230% longer and the system electrical dynamics are about 550% longer.

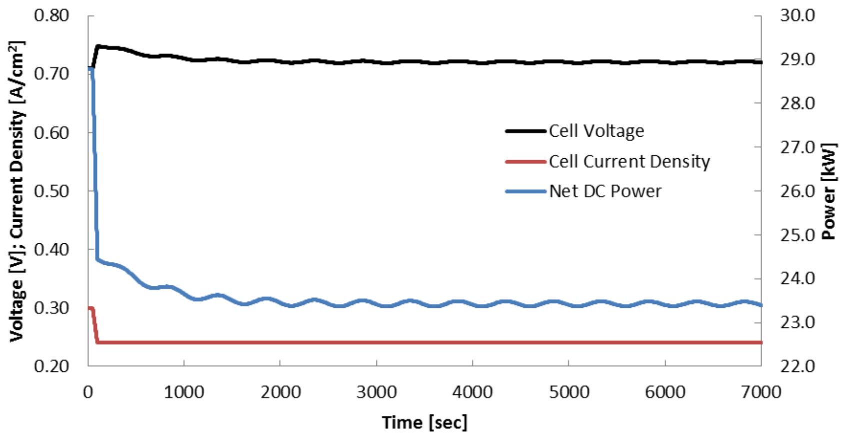

Figure 10: SOFC system electrical dynamics for ramp from 0.3 to 0.24 [A/cm²].

Figure shows the electrical dynamics of the SOFC system for a 50 second current ramp from 0.5 to 0.3 [A/cm^2] with constant fuel utilization and air stoichiometric ratio. This 40% decrease in current load results in a 1% settling time for net power output of 1543 [s] which is only about a minute longer than the 20% reduction case. However, the response is much more defined in its oscillations which are driven by the more dramatic and longer thermal dynamics of the SOFC stack at this higher efficiency operating condition. The results for the 0.5 to 0.3 [A/cm^2] and the 0.5 to 0.4 [A/cm^2] current steps in the stand-alone SOFC cases are not as different as these system results, which signifies that the anode outlet/inlet coupling through AGR and TGC heat recuperation is negatively affecting the thermal and electrical response of the system.

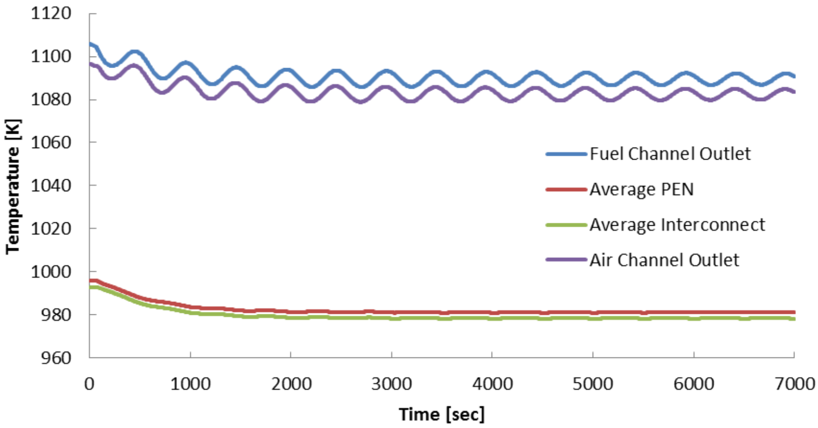

Figure 11: In-system SOFC stack thermal dynamics for ramp from 0.3 to 0.24 [A/cm^2].

The negative impact of recycled stream coupling on system performance is further evidenced in Figure which shows the electrical dynamics of the SOFC system for a 50 second current ramp from 0.3 to 0.24 [A/cm^2] with constant fuel utilization and air stoichiometric ratio. This 20% decrease in current load results in a 1% settling time for net power output greater than 7000 [s]. As seen in the figure, the system is oscillating, seemingly without any dampening at all. The stand-alone SOFC operating under the same 0.3-0.24 [A/cm^2] case was not as oscillatory; however, the system coupling is creating a dramatically under-damped system response. Removing the AGR component of the system or including a bleed valve on the TGC exhaust would help to manage and control this response. Dynamic TGC and heat exchanger models may capture dampening capabilities due to system component thermal mass. Nevertheless, a control system may be required, especially for high efficiency operation such as this. Such oscillation in power output will likely damage the power conditioning equipment that makes the SOFC system and building integration possible.

Figure shows the SOFC stack thermal dynamics for this case. The dampening, however small, is apparent here where the oscillations are slightly diminishing in magnitude with time. The average PEN temperature is oscillating as well, which is undesirable for the stack, where fast and violent dynamics such as this can create thermal gradients that damage the stack and decrease the lifespan of the stack.

Figure further details the system thermal dynamics which are oscillating as the SOFC outlet temperatures are. There is little dampening available for the flow in the SOFC where mass transport is much too fast to dampen the thermal oscillations through the system. The mass of the reformer is again observed to dampen fuel gas temperature oscillations, however the fuel-side recuperative heat exchanger reintroduces these oscillations as evidenced by the fuel channel inlet gas temperature dynamics.

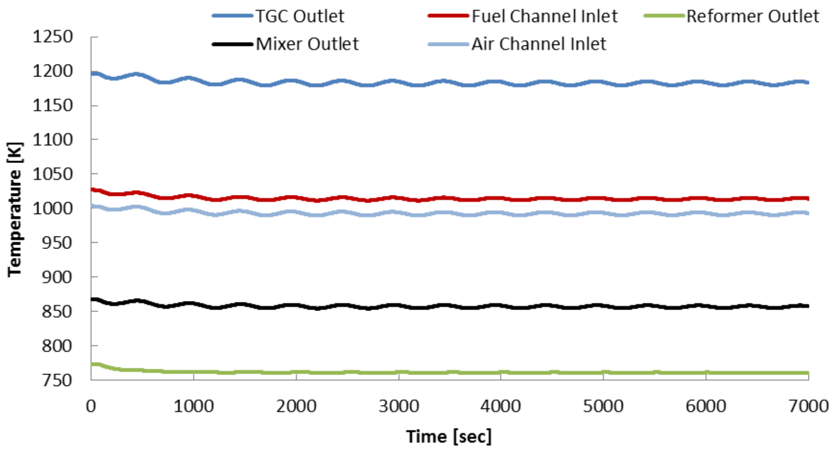

Figure 12: SOFC system flow thermal dynamics for ramp from 0.3 to 0.24 [A/cm^2].

The above SOFC system dynamic analysis shows that the system design amplifies the inherent oscillations of the SOFC stack due to the anode gas recycle / recuperative heat exchanger configuration. The reformer tends to dampen the oscillations of the depleted outlet gas temperature, but the recuperative heat exchanger between the stack exhaust and inlet gas streams is a strong periodic forcing function on the anode and cathode gas stream inlets. As these results are of a preliminary nature and do not include dynamic model fidelity for all system components, numerical simulation errors cannot be ruled out. However, given the low thermal capacitance of the gas streams (i.e., faster response), the theory for the oscillatory gas temperature behavior present at the system-level are logically consistent. Nevertheless, further investigation is necessary to confirm these findings. In terms of commercial building integration, this system design results in highly variable settling times that make the system-building integration problem more difficult than suggested by the analysis of SOFC stack dynamics alone.

3. Conclusion

In this paper a dynamic SOFC system modeling tool for the investigation of dynamic integration for commercial building applications has been presented and demonstrated. The SOFC dynamic stack model developed was one-dimensional, co-flow configuration, and internal reforming capable. Preliminary investigations into the dynamic response of the SOFC stack alone suggest the potential for successful load-following operation in a building integrated application. The average thermal and electrical settling time for the stack was found to be on the order of seven minutes. This dynamic capability is likely to be sufficient for near cost optimal operation. Interesting stack thermal and electrical dynamics were also revealed, as slight oscillations were observed in stack thermal and electrical dynamic response. These oscillations are theorized to be due to a complex coupling between internal solid temperature and current density distributions axially through the cell. In addition, the nature of the stack dynamic response changed according to the efficiency or power output. At high efficiency or low power output, the settling times were longer and oscillations amplified.

The dynamic response of the entire SOFC system was observed to extend for longer time periods and have higher frequency oscillations. The stack thermal and electrical settling times were found to be about 100% and 400% longer in duration when operating within the SOFC system, respectively. In addition, oscillations in system response were shown to be amplified as compared to the stand alone stack investigation. This amplification is thought to be due to the coupling between stack outlet and inlet conditions brought on by anode gas recycle and exhaust gas heat recuperation. Further investigation is necessary to confirm these findings. Interestingly, the thermal capacitance of the adiabatic external pre-reformer serves to diminish the amplitude of the fuel gas temperature dynamics.

A non-linear relationship between system dampening and operating conditions is revealed. This necessitates a control system that can artificially dampen the system temperature dynamics as an SOFC system settling time of over two hours is insufficient for near cost optimal building integrated system operation. In addition, a system redesign may enable faster and more stable thermal and electrical dynamic performance. For example, moving the fuel supply stream reheat heat exchanger upstream of the external reformer would allow for the reformer to dampen the thermal oscillations at the SOFC stack fuel stream inlet. However such conclusions must be supported by analysis of various system configurations and control strategy implementations.

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