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Control of a solid oxide fuel cell system with sensitivity to carbon formation $\dot{\varphi}$

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HIGHLIGHTS highlights are the control of

- < Develops a nonlinear, first principles model of a SOFC system, including all balance of plant components.
- ▶ Reformate composition is modeled and experimentally verified, allows for control of reformer.
- Equilibrium chemistry is applied to calculate reformate quality with respect to solid carbon formation.
- < Novel implementation of a linear parameter varying model reduction.
- < Includes application of model predictive control to a linear parameter varying model.

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Fuel cells allow for increased efficiency in power production when compared to the thermodynamically limited efficiencies of heat engines. In the case of solid oxide fuel cells, they are also usable with the fuel infrastructure currently in place (natural gas). Although potentially transformative, solid oxide fuel cells are currently limited by engineering challenges related to operating temperature (>600 °C), durability, and load following ability. For example, the buildup of solid carbon in the stack, or coking, potentially limits one of the most desirable aspects of solid oxide fuel cells, which is their robustness to fuel type. As the working temperatures for SOFCs continue to decrease, in order to maintain fuel robustness, the need for control of the inlet fuel composition increases. This work demonstrates the use of a model predictive control algorithm on a solid oxide fuel cell system including reformer, blowers, heat exchanger, tail gas burner and stack. The controller allows for load following demand changes from the fuel cell and meets those demand changes, while ensuring that the reformate composition is not prone to solid carbon formation. The controller meets current demand changes to within 0.1 A s^{-1} while maintaining compositional limits on the reformate flow and temperature limits on the stack and reformer.

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1. Introduction

The use of solid oxide fuel cell (SOFC) systems in both portable and fixed installation continues to be the subject of significant research. The high temperatures required for electrolyte conductivity remain an engineering challenge. Current systems employing yttria stabilized zirconia electrolytes tend to operate at approximately 700-800 \degree C. At these high temperatures internal reforming of hydrocarbon based fuels is possible [\[1\]](#page--1-0). However, solid carbon formation, or coking, is still a threat to system durability and robustness. Much current work is focused on lowering the

operating temperatures of SOFC systems. Lower temperatures result in a more efficient electrochemical process and significantly lessen the costs of external components such as blowers, heat sinks, and transport systems. Currently proposed SOFC electrolyte types allow for operation at temperatures as low as approximately 400 \degree C [\[2\]](#page--1-0). At these temperatures external fuel reforming becomes even more important to avoid coking in the stack, as the level of internal reforming is reduced [\[2\].](#page--1-0) The need for external reforming is even greater when biogas is the fuel source [\[3\].](#page--1-0) The goal of this research is to examine if a control algorithm can be designed to control the flow rates of fuel and air to the stack such that the demand current is produced, coking does not occur and the operational limits of the fuel reformer are maintained. The system to be controlled is a potentially mobile 1.5 kW SOFC system. Catalytic partial oxidation (CPOX) reforming has been chosen as it allows faster response times, and the addition of steam is not required. The use of steam or auto-thermal reforming, although more efficient, decreases response time and can be problematic for mobile systems. Air is

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assumed to be available and both fuel and air are moved through the system using blowers.

Control of SOFC systems is challenging due to non-linear system dynamics and the existence of multiple temperature and compositional operating constraints. System components have temperature based operating limits, and the stack has fuel inlet composition and utilization constraints, including avoiding solid carbon formation. Model predictive control (MPC) is a proven control method for meeting constraints, but requires a model that can be optimized in real time. Nonlinear models that capture these constraints are too complex to optimize in real time within a model predictive controller. The approach taken in this work is to create a first principles model that captures the operating constraints, perform a system reduction to obtain a set of linear parameter varying (LPV) models, and implement model predictive control on the resulting LPV model.

The constraints captured include temperatures of inlet and outlet flows from all components, spatially varying temperature of the cell tubes within the stack and heat exchanger and a measure of whether the fuel supplied from the reformer to the stack is prone to solid carbon formation. These constraints provide the motivation for a set of identification operations carried out using the first principles model. This simulation produces input-output data which is then used to identify the LPV model. In effect, the high order non-linear model is used as a simulated experiment to identify the LPV model. The LPV model is actually a set of linear models which are combined or blended using a function of a measured signal. A linear model is calculated at each time step for which the scheduling variable is measured. This linear model is then used to solve the MPC optimization problem to find the new inputs for the system when the controller is implemented.

The proposed method could easily be implemented for any fuel reformer type or stack geometry for which an accurate first principles model exists. Hybrid identification schemes are also possible, where a specific fuel reformer geometry or blower is modeled and used to produce input/output data. The reformer model outputs can then be experimentally simulated and applied to a physical system. The resulting input/output combination can then be used to identify a system wide model for use in model based control. Thermal effects between modeled and experimental components will not be captured for such a hybrid identification scheme.

2. Fuel cell system

The first challenge in developing a model to be used for model based control is determining the level of fidelity. Extremely high order computational fluid dynamics (CFD) models can be created to match very specific geometries and such models capture both the spatial and time varying aspects of the system. Such models are tailored very specifically to the geometries involved and impose a prohibitive computational burden. As such they are most suited as analysis and design tools rather than for control. SOFC systems can also be modeled using lumped thermodynamic models, enforcing mass and energy conservation, but ignoring spatial dynamics and chemical kinetics. Such models also ignore the kinematics at the reformer catalyst and the cells. These effects are important to the operation of the SOFC system and cannot be ignored. Hot spots can occur spatially along cell tubes [\[4\],](#page--1-0) and the reformate composition is highly dependent on the reaction kinetics at the catalyst [\[5\].](#page--1-0) Both these factors impose operating constraints on the system. The model utilized within the controller has to suitably capture such dynamics while still being fast enough that solving an optimal control problem in real time is feasible.

In order to capture the dynamics of the system as closely as possible, we initially develop a non-linear first principles model of the system. This non-linear system model consists of the following (all components are sized for a kilowatt order system):

- Blowers: one to provide air to the fuel reformer, and one to provide air to the stack.
- Fuel reformer: a catalytic partial oxidation reactor which produces the hydrogen rich gas used as a fuel for the stack.
- Fuel cell stack: a collection of tubular solid oxide fuel cells which produces the desired current.
- Tail gas burner: simple burner to combust any remaining fuel products in the stack exhaust in order to help pre-heat air.
- Heat exchanger: a counter-flow tubular heat exchanger to capture heat from the stack exhaust and preheat the stack inlet air.

The blowers are modeled via first principles as in [\[6\]](#page--1-0). The blower model is based off a commercially available blower, an EBM D1G133-DC13-52, which has been rescaled using the fan laws [\[7\].](#page--1-0) The result allows for the calculation of the mass flow as a function of the motor speed and the required pressure differential. Manufacturer data is used to fit a function for the motor speed and the power provided to the blower. No blower is used for the fuel flow to the reformer as it assumed to be under sufficient pressure.

The fuel reformer is considered as a continually stirred tank reactor with surface chemistry. A CSTR was used as it is the lowest dimensional model that can capture the temperature and composition of the reformate. Although a plug flow model would be more accurate, only the final exit composition and temperature are used. The reformer has a tubular geometry with a rhodium catalyst on a foam monolith. The model makes use of the reaction mechanism for natural gas over rhodium developed in [\[5\]](#page--1-0). The model itself has been validated against an experimental CPOX reactor at the Colorado Fuel Cell Center [\[8\]](#page--1-0). Reformate composition and temperature are considered as functions of the input fuel compositions, temperatures and the mass flow rate and temperature of the air provided to the reformer. For the purposes of identification and control the input fuel is biogas with a composition of 70% CH₄ and 30% CO₂. Biogas was used as an input fuel to test the system with a high carbon content fuel, challenging from a coking standpoint. The biogas content was chosen as 70% CH₄ and 30% CO₂ since this composition is within the range of that produced by sewage plants and agriculture. The model, however, fully supports temporal variations in inlet fuel composition and temperature.

The stack model is a combination of high order spatially discretized single tubular cell models. Compositional and temperature variations are captured along each tube length. The model captures heat transfer inside each cell, and from a cell to the gas outside. Thermal effects from cell to cell are not included. To model a stack, 100 tubular cells are connected electrically in series and in parallel with respect to mass flows. The sizes of the tubes are taken as 15 cm long with an outer diameter of 1 cm. The tubular cell model is described in detail in [\[9\].](#page--1-0)

The tail gas burner is simulated using an axisymmetric flame model in Cantera [\[10\].](#page--1-0) The heat exchanger is modeled using a dynamic counter-flow tubular heat exchanger model which allows for varying temperature and composition in the inlet flows. A detailed description of the heat exchanger model is available in [\[11\]](#page--1-0). The physical parameters of the SOFC system are shown in [Table 1.](#page--1-0) Together the system model allows for solutions of the gas flow compositions and temperatures throughout the system. A diagram of the SOFC system and its connections is shown in [Fig. 1.](#page--1-0)

Analysis of the system model provides excellent motivation for the development of an MPC controller to ensure stable and safe operation of the system. For example, with both the fuel reformer and stack air flows supplied via blowers, the dynamic response of the blowers is critical to the ability of the reformer and stack to

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