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# A general approach to develop reduced order models for simulation of solid oxide fuel cell stacks

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## HIGHLIGHTS

- A general approach is provided to develop reduced order models.
- The approach provides rapid calculation with higher fidelity stack information.
- Response surface analysis characterizes the stack over a wide operating space.
- Accurate and efficient response surface generation is based on sensitivity and error analyses.
- Principal component analysis is used to reduce order of state variables.

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## ABSTRACT

Numerical models for solid oxide fuel cells (SOFCs) are needed in system modeling studies of fuel cell-based power generation systems. A reduced order modeling approach based on response surface techniques is developed for SOFC stacks. This approach creates a numerical model that can quickly compute desired performance variables of interest based on the stack's input parameter state. The developed method first carefully samples the multidimensional design space based on the input parameter ranges, automatically evaluates an existing detailed stack model at each of the sampled points, and performs regression for selected performance variables of interest to determine the response surfaces. After error analysis to ensure that sufficient accuracy is established for the response surfaces, they are then implemented in a calculator module for use by the system-level software. The benefit of this modeling approach is that it is sufficiently fast for integration with system modeling software while still providing high fidelity information about the internal distributions of key variables in the fuel cell. This paper describes the sampling, regression, sensitivity, error, and principal component analysis to identify the most appropriate methods for simulating a planar SOFC stack.



## 1. Introduction

The solid oxide fuel cell (SOFC) is a highly desirable energy conversion device [1] due to its high efficiency, high power density, fuel flexibility, ability to support on-cell reformation, low emissions, and production of byproduct heat for cogeneration. Active research is in progress to use the SOFC for large-scale power generation [2,3], as well as distributed generation [4] and even portable transportation applications [5]. A complete fuel cell system requires various hardware components (e.g. blowers, heat exchangers, reactors, combustors, compressors, etc.) that must be carefully integrated for high overall efficiency, so system modeling is critical to define new, cost-efficient plant designs that take advantage of the SOFC's unique features.

These system models must include a mathematical submodel that represents the performance and response of the fuel cell stack, but the submodels used to represent the stack in system analyses typically are only non-dimensional thermodynamic models with a simple mass and energy balance for the entire stack structure. They can compute the stack voltage as a function of single average stack temperature and fuel utilization, but they ignore the influence of any internal distributions. This coarse level of detail is usually selected for its computational speed, as the system model requires many iterations to converge to a steady-state solution or to compute transient changes in dynamic simulations. A fully detailed calculation with stack distributions for species, current density, and temperature usually is too computationally expensive to be used. However, it is

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well known that temperature and current density gradients exist within large stacks [6]. These gradients have important effects on the electrochemical performance, but, perhaps more significantly, the upper and lower temperatures of the cells are not captured. The upper temperature limit usually is a critical design parameter to prevent excessive degradation from thermally activated mechanisms, such as oxide scale growth on the metallic interconnect. The lower temperature limit is important because reduced ionic conductivity of the electrolyte results in poor electrochemical performance that decreases the working voltage of the planar cells. Therefore, models that attempt to capture the distributions within the stack are of high interest [7], and neglecting these dimensional effects can lead to inaccuracy, such as overestimation of the system efficiency [8]. Therefore, a method that provides high fidelity data about the stack distributions with minimal runtime computations is needed to accurately characterize the SOFC operating state in system studies.

While the SOFC conventionally uses $H_2$ as its fuel, it can also utilize carbon-based fuels that contain $CH_4$. The high operating temperature of the SOFC and availability of steam from the $H_2$ oxidation reaction permits direct internal steam reformation of $CH_4$ to $H_2$ on the Ni particles of the cermet anode. This endothermic reformation reaction in the SOFC can be judiciously used for thermal management of large stacks by reducing high temperatures, but inadequate control of spatial reformation on the cell can result in excessive local cooling that can create thermal–mechanical stresses or reduced electrochemical activity. Presently in the U.S., natural gas (whose composition can contain 70–90% $CH_4$) is abundant and inexpensive due to enhanced recovery techniques from shale deposits. Based on continued development of shale resources, the U.S. natural gas supply is expected to grow over the next two decades, and the country is predicted to become a net exporter by 2022 [9]. Low prices, combined with potential cooling benefits, could make natural gas a highly attractive feedstock for future electric power generation. Therefore, the developed SOFC modeling tools should demonstrate the capability to analyze conventional $H_2$ fuels as well as reforming compositions containing $CH_4$.

Numerical simulations for complex systems, such as power generation plants, need to be computationally tractable for general use by the designer; therefore, considerable attention has been paid to reducing the computational cost by developing reduced order models (ROMs) [10–15]. In recent years, reduced order modeling techniques have proven to be powerful tools for various problems, such as circuit design [16,17], software development efforts [18], activation of bacteria [19], aircraft design [20,21], etc. A suitable ROM that closely approximates the high-fidelity SOFC stack models and accounts for internal temperature distributions will be a valuable tool toward improving the accuracy of system simulations that are essential to development and planning for future large-scale, fuel cell-based power plants.

Generally, the problem of model reduction is to replace a given mathematical model of a system or process by a model that is much "smaller" or "simpler" than the original—but still describes, at least, certain aspects of the system or process approximately. Hence, ROMs usually are thought of as computationally inexpensive models that can offer the potential for near real-time analysis [10]. However, ROM construction often is considered as time-consumable and computationally expensive because it requires accumulating a large number of system responses to input excitations [20]. Therefore, an efficient sampling method, sensitivity analysis of input factors and their ranges, and an appropriate regression method are critical to the efficiency and accuracy of the ROM.

The present study proposes a general approach to develop the ROM for simulating SOFC stacks in an efficient manner. In particular, through a sensitivity analysis, we rank the input variables according to their contributions to the sensitivity of each output quantity (see Section 3). The responsive relations are established between the outputs of interest and the inputs through appropriate regression methods (see Section 4). Furthermore, using a recently developed multi-element probabilistic collocation (ME-PCM) method, the distribution of sensitivity is accurately quantified in different regions of input parameter space (see Section 5). Finally, based on the principal component analysis (PCA), outputs with special distributions (i.e., state variables) can be predicted, e.g. temperature distributions within each cell, by establishing an efficient mapping from inputs to their ranked scores (see Section 6). In order to clearly demonstrate the application of the ROM tool to study the SOFC, the proposed approach is mainly applied to a baseline $H_2$-fueled stack using a previously published quasi-two-dimensional electrochemistry model for planar SOFC stacks [6]. The endothermic steam reforming reaction of a $CH_4$ fuel introduces much more complexity to the thermal response of the model, so thorough analysis of reforming fuel compositions and cases will not be presented in this paper. Rather, a fuel composition with $CH_4$ was used with the same model [6] to briefly compare the effect of an alternate reforming fuel composition on the sensitivity analysis.

## 2. SOFC model description

### 2.1. Detailed stack electrochemistry model

A numerical model, called SOFC-MP 2D, was previously developed to simulate the performance of tall SOFC stacks [6]. For symmetric co-flow or counter-flow planar cells where the lateral variations of species, current, and temperature are sufficiently small, a reasonable approach is to consider only the distributions along the flow channel direction and between each series-connected cell. This provides a useful but computationally efficient approach to analyze tall stack towers where significant thermal gradients will develop. This numerical model was used as the demonstration input model for the ROM creation exercise.

The SOFC-MP 2D numerical model consists of an arbitrary number of planar cells composed of the anode-electrolyte-cathode tri-layer, air channel, fuel channel, and interconnect structure. The electrochemical model consists of a one-dimensional approximation applied at each computational point on the iso-potential cell that accounts for the activation, concentration, and ohmic losses based on the local temperature and species concentrations. The flow model solves the species balances for the fuel and oxidant streams, while the thermal model solves the energy balance for the solid and fluid domains, considering conduction, convection, and radiation heat transfer mechanisms. The steady-state results distributions for fuel species, oxidant species, current, and temperature in every cell are calculated, as well as global stack performance metrics, such as current, power, utilizations, peak temperatures, outlet temperatures, etc. For this demonstration model, we focus on a 97% $H_2$ fuel composition, with a 625 $cm^2$ 16-cell stack in a 750 °C furnace environment (denoted as the $H_2$ case for short). For investigating the effect of different fuel composition on sensitivity analysis, a fuel with $CH_4$ was used as well, which contains 11% $CH_4$, 32.4% $H_2$, 33.3% $H_2O$, 4.9% CO, 6.1% $CO_2$, and 12.4% $N_2$ (denoted as the $CH_4$ case for short). The $CH_4$ case was tested in the same cell/stack design as the $H_2$ case. The $CH_4$ case is only used in the input parameter sensitivity analysis as a comparison to the $H_2$ case; all of the remaining analyses (regression for response surface, sensitivity of region of inputs, and prediction of state variables by principle component analysis) are based on the $H_2$ case simulation results.