SOFC MODELING AND SIMULATION
UNDER THE U. S. DOE SECA CORE TECHNOLOGY PROGRAM

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ABSTRACT

The U. S. Department of Energy initiated the Solid State Energy Conversion Alliance (SECA) to facilitate the development of solid oxide fuel cell modules based on mass-customization concepts for use with commonly available fossil fuels at low cost. The U. S. Department of Energy’s National Energy Technology Laboratory and Pacific Northwest National Laboratory coordinate SECA activities. Commercial developers, universities, and government agencies, and other national laboratories participate in the Alliance in a tightly coordinated structure to develop pre-commercial prototypes. The SECA Core Technology Program supports industrial development teams by providing problem-solving research to overcome common technical barriers identified by the industry teams. Core Technology activities include programs in fuel processing, manufacturing, controls and diagnostics, power electronics, modeling and simulation, and materials. The modeling and simulation program develops computational tools to support development and commercialization of SECA technology. This paper reviews the various development and validation activities and availability of modeling tools at DOE national laboratories as part of the SECA Core Technology modeling and simulation program.

INTRODUCTION

The Solid State Energy Conversion Alliance (SECA) of the U. S. Department of Energy (U. S. DOE) was established in the fall of 1999 to foster the development of 3 kW to 10
kW solid oxide fuel cell (SOFC) modules that will be competitive with existing power generation technology, while significantly reducing environmental pollution emissions. The SOFC modules will use commonly available fossil fuels including natural gas, propane, and liquid fuels. Under the SECA program, a government-led project management team coordinates two major program elements; namely, the Industrial Development Teams and the Core Technology Program.

Four industrial development teams have been competitively selected as industry partners to participate in separate cost-shared R&D projects to produce 3 to 10 kW SOFC power generation modules that meet a set of minimum technical performance requirements and cost goals. Systems, manufacturing capabilities, and product packaging needed for different markets will also be developed by these teams. The teams will also deploy balance-of-plant technologies, design elements, and materials needed to achieve breakthrough performance. Industry teams include General Electric Power Systems, Siemens Westinghouse Power Corp., the team of Delphi Corporation and Battelle, and the team of Cummins Power Generation and McDermott Technologies/SOFCo.

The Core Technology Program supports the industrial development teams by providing problem-solving research to address common technical risks and barriers that currently limit achievement of the SECA performance and cost goals for solid-oxide fuel cell systems. The National Energy Technology Laboratory (NETL) and the Pacific Northwest National Laboratory (PNNL) are supplying management and technical resources for the Core Technology Program. The Core Technology program is organized around the following six topic areas:

1. Fuel Processing
2. Manufacturing
3. Controls & Diagnostics
4. Power Electronics
5. Modeling & Simulation
6. Materials.

Within each topic area, needs are addressed for specific science, engineering and technologies, and knowledge and breakthroughs to support development efforts of the SECA industrial teams.

The Modeling and Simulation topic area supports the SECA program by developing and supporting computer-based modeling and simulation tools to help analysis, design, control, and production of high power SOFC modules being developed under the program. The main simulation and modeling activities include:

- System Performance Analysis – overall module and subsystems
- Component Performance Analysis – including cell, stack, reformer
- Stack Component Degradation Analysis – electrical, chemical and mechanical degradation
- Manufacturing Analysis – including economic analysis of module performance
- Material Characterization – measure stack material properties for use in models
- Model Validation – Comparing models to experimental measurements to establish model accuracy and usage limitations.

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System Performance Analysis

System performance analysis tools are used to determine performance of the complete SOFC module, including the stack, fuel processing system, power conditioning, etc. Analysis of the module subsystems is also required to support system design optimization. Systems models can provide the following information:

- overall system configuration
- evaluation of energy transfer and system efficiency
- determine sub-system requirements
- determine system performance at various loads
- evaluate dynamic system performance during start-up and transients
- define and evaluate control system performance and operating strategies.

Component Performance Analysis

Modeling tools are being used to describe the performance of individual components of the SECA modules, including individual cell, cell stack, combustor, and reformer components. These tools can range from simple spreadsheet-based models to detailed models based on computational fluid dynamics (CFD) and finite element analysis (FEA) techniques. Detailed component models can describe the following aspects of component performance for both steady state and transient conditions:

- fluid flow distribution and pressure loss
- overall thermal behavior and heat transfer
- chemical reactions, including combustion, water-gas shift, reforming
- electrochemical behavior for cells and stacks
- stress and strain distribution.

This type of information is critical for design of system components.

Stack Component Degradation and Failure Analysis

Degradation analysis of stack components is necessary to determine long-term performance and reliability of the SOFC modules. Failure analysis aids in establishing criteria for design, fabrication, and operational control. Stack components are subject to both mechanical and electrical/electrochemical degradation mechanisms summarized in Table 1.

Manufacturing Analysis

Modeling of manufacturing techniques is necessary to predict the performance of SOFC module manufacturing plants and to evaluate various fabrication methods and trade-offs. The ultimate goal is to accurately predict the yield and cost of the components based on the relationships between the SOFC design, raw materials, and fabrication techniques used for producing the components. A key objective of this analysis is to understand the effects of design on manufacturing, and vice versa, to enable commercialization of the
technology by providing an accurate estimate of both production and financial performance.

Table 1. Stack Component Degradation Mechanisms.

| Stack Component | Electrical/Electrochemical Degradation | Mechanical Degradation |
|-----------------|---------------------------------------|------------------------|
| Interconnect    | • Increased resistance from oxidation  |
|                 | • Chromium volatility                  |
|                 | • Increased contact resistance         |
|                 | • Material loss from oxidation         |
|                 | • Plastic deformation                  |
|                 | • Contact separation                   |
|                 | • $H_2$ embrittlement                  |
| Anode           | • Ni sintering                         |
|                 | • warping (contact resistance)         |
|                 | • reduced diffusion                    |
|                 | • increased resistance                 |
|                 | • reduced triple-phase-boundaries      |
|                 | • Contamination                        |
|                 | • carbon deposition                    |
|                 | • re-oxidation                         |
|                 | • sulfur                               |
|                 | • silicon/silicate                     |
|                 | • Ni sintering                         |
|                 | • loss of dimensional stability        |
|                 | • cracking in anode                    |
|                 | • interface cracking                   |
|                 | • Interfacial separation               |
|                 | • Damage from thermal gradient and cycling |
| Cathode         | • Increased ionic & electrical resistance |
|                 | • Chromium volatility                  |
|                 | • Susceptibility to Cr poisoning       |
|                 | • Interfacial reaction and diffusion   |
|                 | • Interfacial separation               |
| Electrolyte     | • Aging effects on conductivity        |
|                 | • Damage from thermal gradient and cycling |
|                 | • Loss of gas tight barrier            |
| Seal            | • Electrode poisoning                  |
|                 | • Seal failure and leakage             |
|                 | • Damage from thermal gradient and cycling |
|                 | • Material stability                   |
|                 | • Interface reactions                  |
|                 | • Contact separation                   |

Material Characterization

The modeling and simulation tools rely on accurate values of material properties and understanding how these properties evolve as a function of operating conditions, time, and service history. Properties of interest include transport properties (thermal and electrical), electrochemical properties, and material physical and mechanical properties. The latter include coefficient of thermal expansion (CTE), density, elastic constants,
porosity, tortuosity, strength, and fracture toughness. Many of these properties are difficult to obtain and yet are essential to establish flaw criteria limits to support design and production quality control/assurance processes. Programs are underway at National Energy Technology Laboratory (NETL), Pacific Northwest National Laboratory (PNNL) and Oak Ridge National Laboratory (ORNL) to perform measurements properties that will provide values for various SOFC materials.

**Model Validation**

Comparison of model predictions to other models and experimental data is critical to determine model accuracy. Experimental activities are underway at PNNL and NETL to produce experimental data for validation of component performance models of cells and stacks. Experiments performed at ORNL to study material behavior will supply data for validation of component models predicting stress, strain, degradation, and production flaw criteria. In collaboration with the industrial teams, the predictions of these models, which are probabilistic in nature to address the stochastic nature of the ceramic components in SOFCs, will be compared with actual rates of both infant failures and longer term service degradation rates and failures.

**SIMULATION AND MODELING ACTIVITIES AT PNNL**

PNNL coordinates the modeling and simulation activities of the SECA Core Technology program. In addition, PNNL has an extensive program to develop models for Component Performance Analysis for individual cells and SOFC stacks. In addition, they have supporting programs for Material Characterization and Model Validation. Efforts at PNNL have been focused on the development of new analytical and computational techniques for modeling of rapid-start up, steady state operations, life prediction, and system thermal and electric modeling.

A key feature of the Component Performance Analysis activity is the development of tools that are applicable to a wide range of SOFC designs. The fundamental building blocks of these tools at PNNL are the well-established computational fluid dynamics (CFD) and finite element (FE) analysis codes. Analytical methods are being developed from these basic codes that will provide a complete suite of design tools suitable for SOFC fuel cells. These tools cover the full range of design criteria, from rapid start-up to steady state operations to life predictions. These tools range from simple data translation routines to translate CFD thermal results to a FE structural grid to complex algorithms that predict electro-chemical heat generation at the micro-structural level. The suite of tools available at PNNL includes

- transient thermal-fluids stack model
- structural model of rapid start-up SOFC operation
- thermal-fluid-electrochemical modeling of steady-state SOFC operation
- electrochemical modeling of steady-state SOFC operation using the finite element method
- thermomechanical data for seals and interfaces.

We will limit the discussion to first 3 sets of models listed above.
**Transient Thermal-Fluids Stack Model**

During fast startup or fast cool down, thermal stresses that develop within the fuel cell stack must be maintained below an acceptable level. The stresses are a consequence of CTE mismatch, temperature gradients, and stack structural loads. It is necessary then to model the flow of heat and mass transfer through the fuel cell stack to describe the transient temperature distribution. The predicted transient temperature distributions computed by CFD models are used as input to the FEA code to predict the thermal component of the stress. Knowledge gained of the stress in the stack can be used to establish control parameters during transient operations and establish limits for structural loads.

The thermo-fluids modeling of the fuel cell stack is being performed using the commercial CFD code, Star-CD. Sub-models containing the full geometric detail of individual interconnect features, such as a single air flow channel, calculate the pressure drop and heat transfer coefficient for particular channel and interconnect dimensions. These conditions are imposed in the full stack model. The full stack models are then able to solve the bulk flow and heat transfer conditions. With this approach, similar configurations can be tested parametrically using a single full-stack model. These full stack simulations are an extension of the single channel models; therefore, the material properties remain the same.

Several start-up simulation cases were run using single model geometry. This geometry is shown in Figure 1. The upper left portion of Figure 1 shows the full stack geometry. The air (cathode) outflow manifold is sized larger than the inflow manifold to ensure uniformity of flow throughout the stack height. Heating air is introduced at the bottom left hand side of the stack (narrower manifold), travels across the interconnect channels, and exits downward at right (wider manifold). The “zoom” view of the stack at upper-right in Figure 1 shows more detail of the grid. Details of the individual flow channels are simulated using a porous media model in the active area. This 3-dimensional model contains 470,000 computational cells. We have investigated several stack designs and will present results for a representative design. Thermal stack simulation for this case reached operating temperature of 700°C in about 25 minutes. Thermal gradients in the cell were significant (230°C or less within each cell). Figure 2 shows the temperature distribution in a cell at 25 minutes. The maximum temperature occurs at the inlet cathode side of the cell.

Several design options for minimizing the temperature and stress gradients were investigated. One option studied heating the outer wall of the stack. While this design option assists in transferring heat to the stack, it does not provide enough heat to reduce thermal gradients within the stack during rapid startup. Temperature control of the inflow and stack wall temperature allows start-up time to be minimized while avoiding excessive thermal stresses. Simulations of shorter, less massive stacks show promise for achieving the goal of rapid start-up with acceptable thermal stresses.

**Structural Model of Rapid Start-up SOFC Operation**

The temperature distributions at a given time, obtained from CFD analysis, were then used to calculate the stresses in the stack. An FEA model was generated using ANSYS.
to predict mechanical failure that could result from excessive stresses due to the mismatch of thermal expansion coefficients of the cell materials. Each cell consisted of cell (cathode, electrolyte and anode), cathode and anode spacers, interconnect, and glass seals. The Young’s moduli and the thermal expansion coefficients of the component materials were assumed to be temperature dependent, while Poisson’s ratios were assumed constant. All of the materials were assumed to be isotropic.

The failure criterion adopted here is based on the strength of the cell materials and the principal stresses developed by the thermal loading. To visualize the stress concentration in the interconnect, von-Mises equivalent stress is calculated and compared with the yield strength of stainless steel 430 series. It is possible that crack initiation and propagation can occur along the interfaces between the components, but the study of interfaces is beyond the objective of the current study. The cathode and anode spacers were 430 stainless steel, and the same material properties as interconnect were used. It should also be noted that the cell structure was modeled as 3 layers (i.e. the anode, electrolyte, and cathode).

The ANSYS model was built using 8-node solid brick elements. To generate a 3-D model, a 2-D “footprint” that had all the necessary areas and boundary lines to represent every component in the cell was made in advance. The same footprint would be used for both CFD and FEA models so that the temperature data could be transferred from CFD to FEA seamlessly. The footprint was then expanded to a 3-D model for a 3-cell fuel cell stack. One cell is composed of a metal interconnect (75 μm), an anode spacer, a cell, and a cathode spacer. Mesh refinement was used where large stress gradients were expected, such as around the corners.

A finite element model of a three-cell stack was constructed. Unlike the cell model shown in Figures 1 and 2, the cell PEN for this transient stress simulation is modeled explicitly as a layered structure. The highest stress in a stack cell was observed at the air outlet side. The maximum principal stress in the anode was 82 MPa. High stress also occurred at the corner radius of the air inlet manifold in the metal interconnect as shown in Figure 3.

**Thermal-Fluid-Electrochemical Modeling of Steady State SOFC Operation**

A simulation tool for three-dimensional modeling of planar solid-oxide-fuel-cells has been demonstrated. The tool combines a commercial thermo-fluids simulation code and a validated electrochemistry calculation method (4) enabling the calculations to be performed on complex, 3-dimensional meshes. The effects of cell flow configuration on the distribution of temperature, current density, and fuel species was investigated. For example, we will show results for three flow configurations, cross-flow, co-flow, and counter-flow using identical inflow rates and temperatures. Some results from the three flow configuration cases are shown in Figures 4, 5, and 6. Temperatures are shown in Figure 4. Current density is shown in Figure 5. Mass concentration of the carbon monoxide is shown in Figure 6. The cross-flow PEN temperature distribution is shown in plan view in Figure 4a along with co-flow (Figure 4b) and cross-flow (Figure 4c). In each case, the temperature, plotted on the same scale, increased along the air flow direction reaching a maximum near the air exit. Of the three flow configurations tested, the co-flow case had the most uniform temperature distribution and smallest difference in
temperature from air inlet to air outlet. This is due to air near the inlet, at its coolest, being aligned with the fuel inlet where Nernst potential is highest. Counter-flow showed the largest difference in temperature across the PEN. Consistent with the temperature distribution, the current density in Figure 5 was most uniform in the co-flow case. In the cross-flow and counter-flow cases, current density is high near the fuel inlet and air outlet corresponding to high temperature and Nernst potential in that region. This result was not present in the co-flow case where the maximum current density was roughly midstream from inlet to exit.

Mass concentration of CO is shown for the three cases in Figure 6. The primary difference is the strongly 2-dimensional character of the cross-flow case. While the co-flow and counter-flow cases have low fuel concentration across the full width of the fuel outlet, the cross-flow case has a “point” minimum. When trying to maximize fuel utilization, this characteristic would be undesirable due to increased risk of localized fuel depletion. This tool and others are being used to assist in design optimization of cells and stacks for optimum performance. Parameters being optimized include cell performance at high fuel utilization, uniformity of gas flows, and thermal and mechanical stress profiles during stack operation and startup/shutdown.

EXPERIMENTAL ACTIVITIES AT ORNL IN SUPPORT OF MODELING AND SIMULATION

ORNL has initiated an experimental program to measure physical properties of stack components. ORNL is in the process of identifying and using various techniques to determine the elastic properties of electrodes and electrolytes. These techniques include resonant ultrasound spectroscopy, impact excitation and nano-indentation.

Measurements are being made to determine the in-plane biaxial strength of electrodes and electrolytes, because the dominating stresses will be of the in-plane type for the planar cell geometry. ORNL has also developed test fixtures to evaluate the biaxial strength of SOFC components at room and elevated temperatures and in controlled environments using the ring-on-ring test method. These strength measurements are being complemented with thorough fractographic analyses to identify the characteristics of strength-limiting flaws. The results from these tests and analyses will provide material producers with information to enable modifying the material or the synthesis process in order to eliminate unwanted strength-limiting microstructural features and defects. Because many SOFCs have to be sintered in air, anodes are not reduced until the SOFC is subjected to operation. Therefore, the ability to evaluate the mechanical and physical properties of various SOFC components in controlled environments is essential to understand how the microstructure and properties of these materials evolve with the environment. Furthermore, the results from these tests will provide the appropriate values of their properties for the calculation of stresses and reliability.

To support the industrial teams in the optimization of SOFC designs and behavior, ORNL is currently investigating the effect of porosity and thickness on properties of anodes and electrolytes. ORNL is also developing non-destructive techniques, based on ultrasonics and infrared imaging, to correlate the distribution of defects in SOFC materials and components with their mechanical and physical properties. However, the ultimate objective of the work at ORNL is to develop methods to predict the reliability and...
durability of materials and components for SOFCs. Like most complex systems, the failure rate of SOFCs as a function of service time can be described by a "bathtub" curve as illustrated in Figure 7. Some components will fail relatively early (infant mortality failures). Most will last until they wear out, and some will fail during the relatively long period typically associated with normal life. Failures during infant mortality are highly undesirable and are always caused by material and manufacturing defects, design shortcomings, errors in assembly, etc.

ORNL is supporting the industrial teams by helping them to identify the type and characteristics of defects that are responsible for infant mortality failures. Because the strength of ceramic materials is stochastic in nature, the development of models to predict infant mortality rates in SOFCs will be based on the use of probabilistic methods. Currently, ORNL is utilizing the CARES (Ceramic Analysis and Reliability Evaluation of Structures) methodology to predict the early-life reliability of SOFCs by combining the temperature and stress distributions obtained by detailed SOFC models from NETL and PNNL and experimental results from the mechanical evaluation of SOFC components. The steps involved in determining the probability of failure are illustrated in Figure 8.

SIMULATION AND MODELING ACTIVITIES AT NETL

NETL has large programs to develop models for Component Performance Analysis for individual cells and SOFC stacks and for Model Validation. A detailed model of the solid oxide fuel cell (SOFC) has been developed by modifying the FLUENT™ commercial computational fluid dynamics (CFD) package (1,2). The FLUENT™ CFD code is a finite volume-based code solving the conservation laws of mass, energy, momentum and electrical potential in an unstructured mesh. The SOFC model calculates fluid flow, chemical species transport, heat transfer, electrical potential field, gas-phase chemistry, and electrochemistry in a three-dimensional SOFC geometry for steady-state operation. Fluid flow calculations include the effect of porous electrode regions on flow behavior. Chemical species transport models include multicomponent diffusion through porous regions. The temperature data from the SOFC model has been coupled to the ANSYS finite element analysis code to determine thermal stresses in SOFC components.

The NETL SOFC model is composed of the following custom capabilities

- electrochemical submodel
- electrical field submodel
- mass diffusion in porous media

The model has also been recently extended to model SOFC stacks. Validation of the stack modeling capability is underway.

NETL has also developed experimental facilities to generate data for validation of the SOFC model. Well-characterized SOFC test specimens are being tested in fuel cell test stands for single cell and short-stack arrangements. Anode-supported cells with controlled electrode microstructures, electrode thickness, and electrolyte thickness will be tested. Operating data from the test stands will include cell and stack polarization curves,
temperature data, and chemical composition of reactant streams. Figure 9 shows one of the NETL experimental rigs, four of these rigs are presently in service.

**Validate Models with Experimental Data**

NETL is constructing an SOFC test facility to test small cells and short stacks. This facility will generate detailed data for well-characterized SOFC test specimens operating under a broad range of conditions. Collaboration is now underway with the University of Utah, Department of Materials Science and Engineering. The University of Utah will provide anode-supported test specimens for the NETL facility. The standard test specimen has the following configuration:

- YSZ electrolyte, ~7-10 microns thick
- LSM+YSZ interlayer, ~20 microns thick
- LSM cathode layer, ~50 microns thick
- Ni + YSZ interlayer, ~20 microns thick
- Ni + YSZ anode support layer, ~1mm thick

Cells with range of anode thickness, electrolyte thickness, cathode thickness, and anode porosity will be studied.

Preliminary results for a standard test cell have been generated. The cell is supplied with 95% H₂, 5% H₂O as fuel, operating at a cell temperature of 800°C. Oxygen in ambient air is supplied as the oxidant. An example of the NETL test rig and the comparable CFD computational domain is illustrated in Figure 10. The cell is mounted in ceramic flanges with mica gaskets and inserted in a tube furnace. Furnace heat input is adjusted in the model to maintain constant cell temperature.

Figure 11 illustrates the comparison between measured and predicted performance curves, both voltage and power density as a function of cell operating current. Good agreement is exhibited between data and model over the whole operating range indicating that the model accurately represents SOFC physics.

**Future Work**

PNNL developed tools for optimizing stacks for both rapid start-up and steady-state operations and can address various stack configurations and fuels. PNNL has also recently released a stand-alone thermal systems modeling program in a Microsoft Excel framework. All of these tools are available to SECA industrial team members. In the near future, PNNL will be working to supply these tools to interested SECA industrial development teams and to support their use of these tools. PNNL is currently extending the capabilities of the steady-state modeling tools and is developing microstructural electrochemistry modeling tools.

NETL will extend the electrochemical models to study transient operation and parallel processing for increased simulation speed. Further validation will be performed using data from the NETL SOFC test facility and from collaborations with SECA Industrial Teams.
The mechanisms that are responsible for time and service-dependent degradation and that promote the growth of strength-controlling defects will be identified and characterized. Mechanisms such as sintering, slow crack growth, thermal shock, thermal fatigue and creep are expected to play an important role in the degradation of SOFC components. This information will then enable the formulation of models to predict failure (reliability and durability) as a function of time and service history.

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Figure 1. Thermal-fluids stack model geometry.

Figure 2. Predicted cell temperatures (contour range 600°C–800°C)
Figure 3. Equivalent stresses in stainless steel components.

Figure 4. PEN temperature (C) for (a) cross; (b) co-, and (c) counter-flow.
Figure 5. Current density (A/cm²) for (a) cross; (b) Co-, and (c) counter-flow.

Figure 6. Contours of mass fraction of CO (kg/kg) in fuel stream for (a) cross; (b) co-, and (c) counter-flow
Figure 7. Bathtub Curve for Failure Rate

Figure 8. Steps to determine probability of failure of SOFC cell and stack.

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Figure 9. NETL SOFC test rig.

Figure 10. NETL SOFC button cell test rig and CFD geometry.
Figure 11. Comparison of measured and predicted standard cell performance.