IV.J.2 Modeling and Control of an SOFC APU

Moe A. Khaleel (Primary Contact), Brian J. Koeppel, Ba Nghiep Nguyen
Pacific Northwest National Laboratory
P.O. Box 999, MS K2-18
Richland, WA 99352
Phone: (509) 375-2438; Fax: (509) 375-6605; E-mail: moe.khaleel@pnl.gov

DOE Technology Development Manager: John Garbak
Phone: (202) 586-1723; Fax: (202) 586-9811; E-mail: John.Garbak@ee.doe.gov

Objectives

- Task 1: Develop dynamic system model of a solid oxide fuel cell (SOFC) auxiliary power unit (APU) and design a system controller to minimize diesel fuel consumption, to maximize operating lifetime, and to satisfy electrical load requirements for Class VIII truck applications.
- Task 2: Develop analytical models and perform testing to determine the dynamic structural response and vibrational limits of SOFC-based APU systems in a Class VIII truck operational environment.

Technical Barriers

This project addresses the following technical barriers from the Fuel Cells section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

- C. Thermal Management
- D. Fuel Cell Power System Benchmarking
- H. Startup Time
- P. Durability

Approach

Task 1

- Create dynamic operational models for the SOFC stack, power electronics, and balance-of-plant components using first principles and experimental data.
- Create system functionality model by combining component models in Simulink.
- Design controllers using model to optimize fuel efficiency and lifespan.
- Ensure models and controllers are realistic through experimental testing and collaboration (e.g., collect electrical load profiles with PACCAR and test APU systems with Delphi).

Task 2

- Develop a lumped parameter model to determine the vibration amplitude of the SOFC stack due to base excitation of the APU.
- Perform stress analysis on using a detailed finite element model of a multiple-cell planar SOFC stack and the stack loading history.
- Develop failure models for positive-electrolyte-negative (PEN) fracture and seal interfacial separation to define APU vibrational limits and isolation requirements for stack durability.
- Perform experimental testing to collect actual vibration loads of a truck-mounted APU and validate dynamic models.

Accomplishments

Task 1

- Added secondary storage model of battery and a controller to supplement stack electrical output when load demand is high.
- Added an operating controller that adjusts flow rates as stack current varies to maintain constant fuel utilization.
- Performed experimental testing on an operating SOFC to determine dynamic response to load variations.
- Added improved power electronics system model comprising a state-space averaged model of a DC-DC converter through collaboration with University of Illinois.

Task 2

- Developed transient and spectral methods to analyze shock effects on stack model.
- Developed a modified boundary modeling (MBL) approach using ABAQUS to efficiently predict fracture toughness and crack resistance behaviors of APU SOFC materials, particularly brittle glass seals.
- Developed a method based on MBL modeling to numerically predict fracture toughness of interfaces between layer materials.

Future Directions

Task 1

- Optimize controller performance based on interactions between the cell, power electronics, and balance-of-plant.
- Improve the transient thermal response of the stack model.
- Collect typical electrical system load profiles in Class VIII trucks with PACCAR.
- Work on higher level control techniques to improve overall system efficiency.

Task 2

- Develop a continuum fatigue damage model for cyclic loading and validate with experimental data.
- Integrate damage model into stack analysis to determine cyclic loading limits for rigid glass seals.
- Define APU isolation requirements for various SOFC and APU designs.
- Perform experimental testing to obtain actual truck vibration data and validate model predictions of APU response.

Introduction

Long-haul trucks require electrical power to operate hotel loads while parked for the operator to rest. Typically, these loads are powered by idling the engine or a dedicated diesel generator-based auxiliary power unit (APU). Fuel cell based APUs hold the promise of greater energy efficiency, lower operating costs, lower emissions, and quiet operation. An SOFC is expected to be the choice for transportation applications because: 1) it has higher power density than other designs to minimize stack mass and volume, and 2) it offers fuel flexibility due to its high operation temperatures and toleration of impurities.

This project looks at modeling of SOFC APUs to understand how design choices impact efficiency and durability. Task 1 investigates operational models of APU components and the entire system to show how the devices interact and allows different configurations to be investigated for increased fuel efficiency. The operational models will be used to create effective control strategies to optimize fuel efficiency and lifespan. High temperatures and dissimilar materials severely impact SOFC structural robustness, and the rigorous dynamic loading of a heavy truck makes it even more challenging. Task 2 provides modeling tools to evaluate the thermal-mechanical stresses in the stack under quasi-static and dynamic conditions. This will allow designers to define appropriate materials, cell design, physical layout, and isolation components to minimize vibrational loads to acceptable levels for increased durability of SOFC APUs.

Approach

Task 1: The approach to creating operational models of the APU components and system has been to combine theoretical operation with experimental data, keeping the models broadly applicable but realistic. Electrical load profiles from Class VIII trucks will be collected with PACCAR to understand how APUs are used in practice. Models for components such as the diesel reformer, heat exchangers, power electronics system, battery, and SOFC stack are created in the modular Simulink environment that allows them to easily be connected in different configurations. This allows different fuel and thermal management strategies to be tested. Work on the controllers, with independent control of individual components, has begun. This will be followed by higher level controllers, coordinating all components and increasing fuel efficiency. Finally, as the model matures, it will be possible to optimize control to minimize fuel consumption, maximize lifespan, and meet electrical load requirements.

Task 2: The APU system was modeled at three different levels. Previously, a lumped parameter representation of the APU and a detailed stack model were developed to compute the deformation and stresses of the cells due to dynamic loading. Stress analysis results are used in conjunction with failure criteria to define allowable excitation amplitudes. Damage and interfacial crack growth in rigid seals is expected to be of primary concern for cyclic loading of the stack. Since damage and fracture processes occur at scales which are much smaller than those of a fuel stack or system, it is essential to understand and analyze the damage and fracture processes at the *micron-scale*. To this end, the third model uses a modified boundary layer (MBL) modeling approach developed to predict the fracture toughness and crack resistance behaviors of SOFC materials. In this approach, a pre-existing crack inside a layer or at an interface between two different layers is assumed under plane strain conditions. Fracture is allowed to occur in a small process window situated at the crack tip. The process window, whose size is about several tens of microns, is contained in a circular region, which can involve one or two different materials and their interfaces. Elastic asymptotic crack-tip fields are prescribed as remote boundary conditions. Special attention is focused on the cracking of the interface between the glass seal and the electrolyte material. The advantage of the MBL analysis is that it can be used efficiently to characterize the material and interface toughness as well as the crack resistance behavior without knowing the exact geometry of the structure and the associated boundary conditions. These results will be used with the stress analysis results and parametric analyses to define allowable excitation amplitudes. Collection of actual excitation loads and experimentally testing the SOFC components and APU will validate the models.

Results

Task 1: The system model created in the prior year has been improved. First, the stack operating controller was improved to maintain constant fuel utilization for desired efficiency. As the electrical current changes, the controller modifies the anode gas flow. Second, a secondary storage device was added to the APU system. Using a battery allows the APU to run at higher fuel utilization for efficiency but still meet high electrical load demands and transients. An accompanying controller was also included to increase SOFC output when required to provide excess power for maintaining battery charge. Third, the transient electrical response of the fuel cell was experimentally measured. The load for an operating SOFC was varied to study the stack dynamic response at temperatures of 700-800°C (Figure 1). The data was fit to a transfer function of the following form:

$$\frac{V_{oc} - V_{out}(s)}{I(s)} = \frac{R_a R_{ohm} C_{cdl} \cdot s + R_a + R_{ohm}}{R_a C_{cdl} \cdot s + 1}$$

where

V_{oc} = open circuit voltage

R_{ohm} = ohmic resistance through cell

R_a = activation loss, caused by slowness of reaction

C_{cdl} = charge double layer effect capacitance

I = electrical current

s = Laplace variable

The resulting parameters are shown in Table 1. Finally, the power electronics system model was improved through collaboration with Sudip Mazumder of the University of Illinois. The new model is a state-space averaged model of boost DC-DC converter. The transient model operates under closed loop control, which can be either a single-loop current controller or a multi-loop controller which regulates bus voltage and current simultaneously. The performance of the power electronics system with the multi-loop controller is shown in Figure 2. The power electronics model is currently being integrated into the SOFC system model.

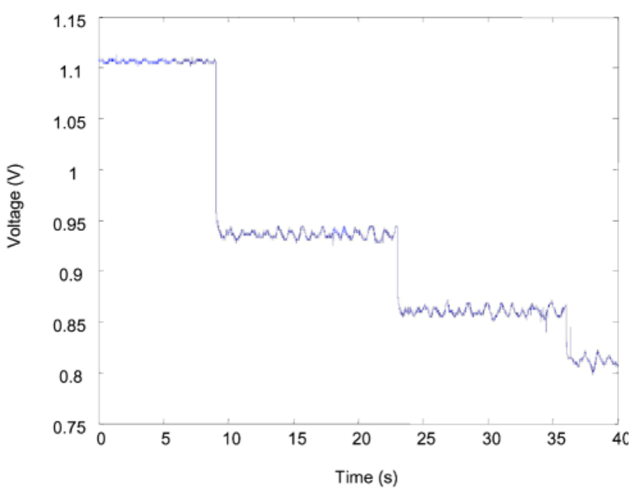

Figure 1. Experimental Voltage Response of Single Cell SOFC (Each transition indicates a load change in the test circuit to see the I-V relationship at three distinct current levels.)

Table 1. Parameter Values for Transient Response Function

	700C	750C	800C
Voc	1.11	1.11	1.10
Rohm	0.0264	0.0247	0.0167
Ra	0.0147	0.01	0.01
Ccdl	7.1	7.1	13.8

Task 2: Several enhancements were made to the previously developed models which compute stack stresses based on thermal and dynamic loading. The capability to model shock events was added using transient, equivalent static load, and spectral methods. Additional tensile stress, fracture, and displacement based criteria were added to the model for the anode, electrolyte, cathode, and glass seals, based on experimental data from the literature and the SECA Core Technology Program. The union of all the potential failure criteria defines the limiting

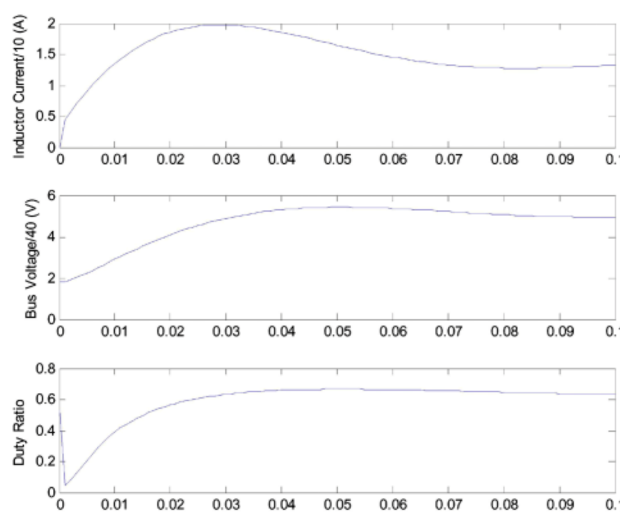

Figure 2. Performance of the power electronics system model including (a) “scaled” inductor current, (b) bus voltage, and (c) duty ratio. An initial bus voltage of 72 V is assumed to speed up the simulation. For a load of 1000 W, the value of the inductor current at steady-state should be close to 1000/72 = 14 A. The bus voltage for this simulation is being regulated at 200 V. The duty ratio in steady state should be

$$d = 1 - \frac{72\ V}{200\ V} = 0.64$$

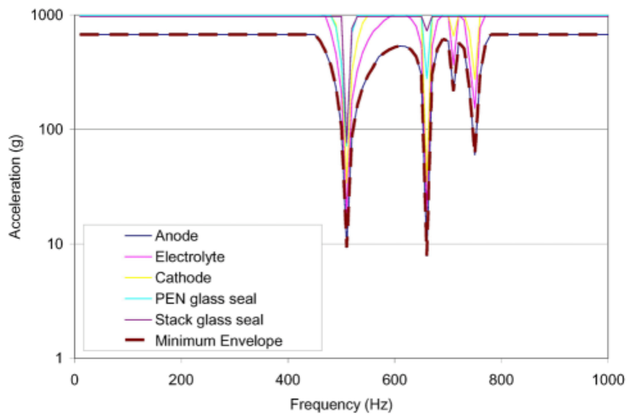

Figure 3. Permissible Acceleration Envelope for the Planar Stack Developed from Multiple Cell Failure Criteria

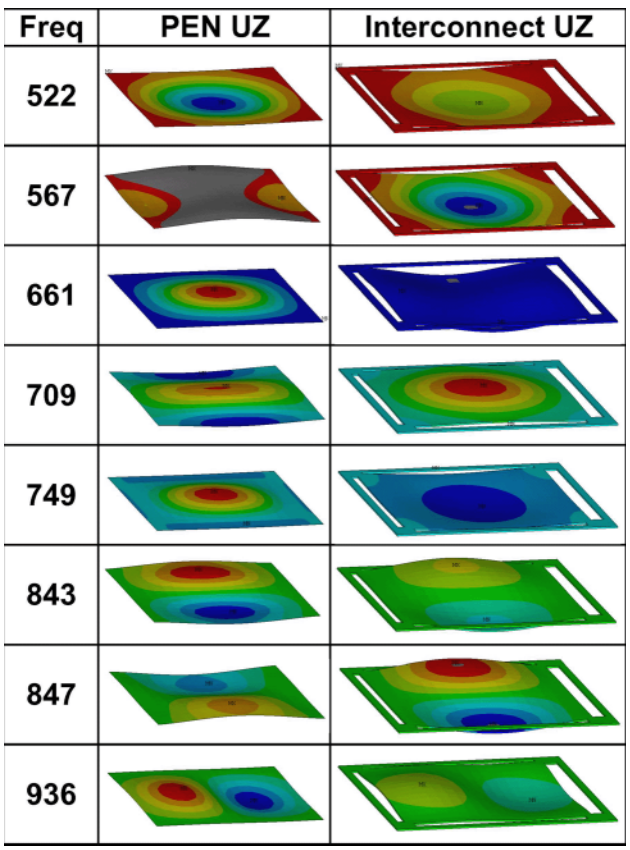

Figure 4. Modal Frequencies for the Planar SOFC Stack, where Modes 1, 3, 4 and 5 are Excited

acceleration envelope for the stack (Figure 3), where the critical frequencies identified through modal analyses are the frequencies of interest (Figure 4). The influence of excitation direction

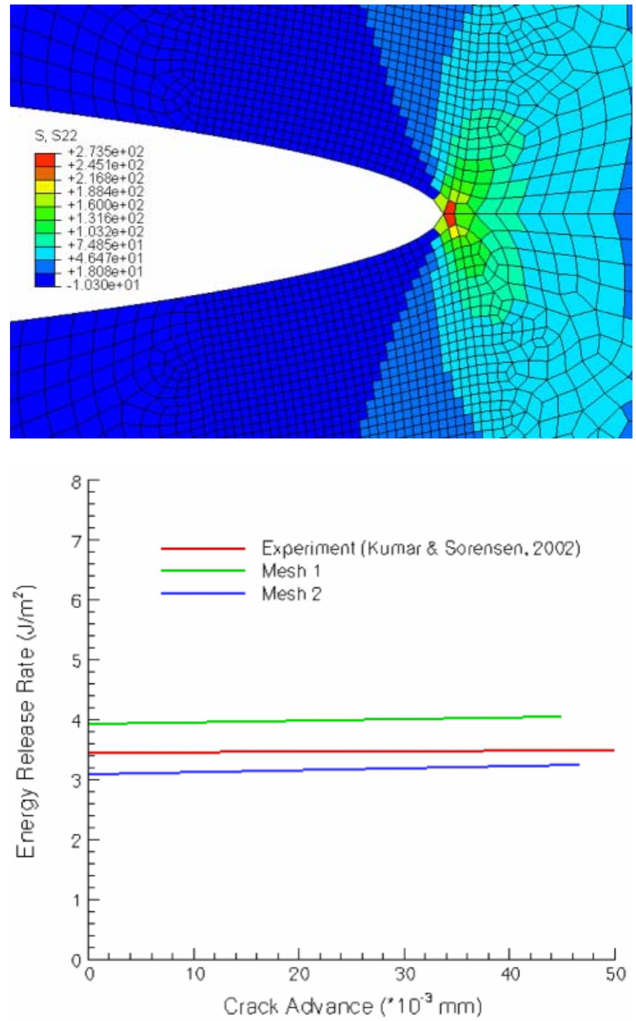

Figure 5. (**a**) Contour of the Crack Opening Stress for a Crack Advance of 0.046 mm (**b**) Predicted and Experimental Energy Release Rates versus Crack Advance for the YSZ Material used in [1]

and damping was also investigated. The main structural integrity problem is expected to be interfacial separation of the rigid seals which is being studied with the MBL model.

The MBL model was validated using the material properties found in literature for the YSZ material [1], and the experimental data for the G18 glass seal determined at PNNL. In this report, the predictions of the fracture toughness and crack resistance behavior of the YSZ material used in [1] are illustrated. Figures 5a shows a crack propagation stage in the process window for a crack advance of 0.046 mm while Figure 5b presents the predicted crack resistance curves expressed in terms of the energy release rate as a function of the crack advance for the YSZ material at 20^{o}C. Two different meshes were used for the analyses. The experimental results show no crack resistance ability for this material. Such a behavior was modeled by imposing the stresses to be relaxed immediately after the failure criterion had been satisfied. The average experimental curve from [1] is also presented in Figure 5b that shows a good agreement of results both in tendency and numerical values.

Next, the focus was placed on the interface crack problem. According to Rice [2], the interface crack-tip stress field is governed by the complex stress intensity factor, the mode mixity and the properties of dissimilar materials. Among these parameters, the mode mixity has a strong effect on the interface fracture toughness. The MBL modeling was used here to numerically establish the fracture toughness/ mode mixity relationship that is highly important for design of fuel cell stacks, in particular the design of glass seal/electrolyte interfaces. It is noted that the mode mixity is linked to a reference length whose choice is based on a material length scale such as the size of the fracture process zone, the zone of dominance of the crack-tip field, etc. Figure 6a illustrates the variation of the normalized fracture toughness $|\boldsymbol{K}_c|$ with the mode mixity ψ_0 for an interface crack between the glass and YSZ materials. The minimum value of $|\boldsymbol{K}_c|$ occurring at $\psi_0 = 23^o$ for which the contribution of Mode II is minimum was used as the reference value for the normalization. For $-35^o < \psi_0 < 23^o$ and $23^o < \psi_0 < 90^o$, there is strong increase in toughness with increasing contribution of Mode II to the loading. Figure 6b shows the opening stress profile around the crack tip for the case $\psi_0 = 69^o$ where the stress field is strongly governed by Mode II.

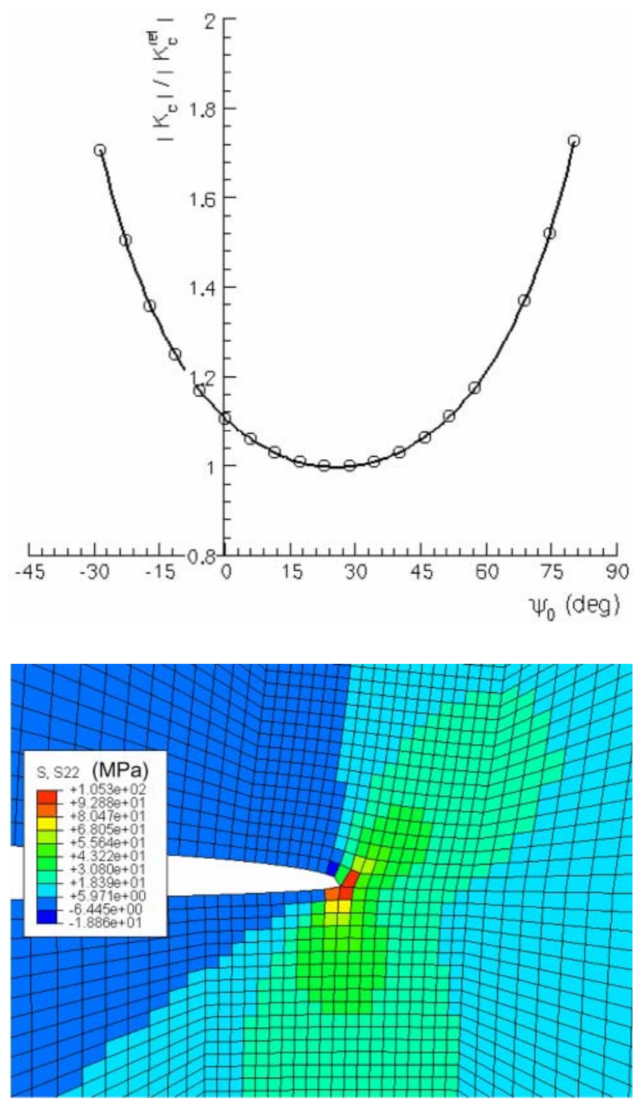

Figure 6. (a) Glass/YSZ Interface Toughness as a Function of the Mode Mixity ψ_0 (b) Opening Stress Profile at the Onset of Crack Propagation for the Case $\psi_0 = 69°$

Conclusions

- Task 1: State of the art models of an SOFC APU system and components were developed to describe the operational behavior of the APU. The models were used to develop controllers to provide required current and maintain fuel utilization under varying electrical loads. Experimental tests on a single cell SOFC determine its electrical transient response, and the resulting transfer function was used in the stack model. A detailed power electronic model was provided by the University of Illinois and incorporated. Further controls tuning will be done based on the interactions of the fuel cell, power electronics, and balance-of-plant components.
- Task 2: Finite element models were constructed for vibration and shock analyses of an SOFC-based APU with various failure criteria to predict permissible vibration load as a function of

frequency. The effects of load direction and material damping were investigated. To study interfacial behavior, the developed MBL modeling approach is efficient and practical since it allows the fracture toughness and crack resistance behavior of SOFC materials to be directly estimated. In particular, the numerically established interface toughness/mode mixity relationship is very useful for the design of sealing materials in SOFC stacks. The approach only requires a few material data inputs such as the elastic properties and failure stresses, although it does require knowledge of the material microstructure (e.g. grain size) for the mesh size criterion for the process window.

References

1. A.N. Kumar and B.F. Sørensen, "Fracture Energy and Crack Growth in Surface Treated Yttria Stabilized Zirconia for SOFC Applications," *Materials Science & Engineering A,* **A333** 380-9 (2002).

2. J.R. Rice, "Elastic Fracture Mechanics Concepts for Interfacial Cracks," *Journal of Applied Mechanics*, **55** 98-103 (1988).

FY 2004 Publications/Presentations

1. M.A. Khaleel, B.J. Koeppel, and S.J. Moorehead, "Modeling and Control of a Solid Oxide Fuel Cell Auxiliary Power Unit," Hydrogen, Fuel Cells & Infrastructure Technologies Program 2004 Annual Review Meeting, Philadelphia, PA (2004).

2. B.N. Nguyen, B.J. Koeppel, S. Ahzi, P. Singh, and M.A. Khaleel, "Numerical Characterization of the Fracture Behavior of Solid Oxide Fuel Cell Materials by Means of a Modified Boundary Layer Model," Proceedings of the 28th International Cocoa Beach Conference on Advanced Ceramics and Composites, Vol. 25, Iss. 3-4, (2004).