Temperature and Stress Distributions in micro-Tubular SOFC (107)

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Motivation

The runtime of mobile robotic platforms can be greatly increased using Solid Oxide Fuel Cell (SOFC) stacks fueled by readily available propane and hybridized with lithium ion batteries. However, SOFC systems suffer long-term degradation due to thermal cycling during startup and shutdown. The operating temperature range of the SOFC is around 800 to 1100 ^{o}C. The aim of this study is to understand the factors that influence the lifetime of micro-tubular Solid Oxide Fuel Cell (mSOFC) stacks. Three-dimensional models are developed to investigate the effect of operating conditions and temperature distribution on thermal stresses and electrical performance of mSOFC. The simulation results provide information about the location and magnitude of stresses for a given cell design. In addition, the sensitivity of axial and radial Von Mises stresses are analyzed using various temperature profiles. The model can be used determine the limit of thermal gradient induced stresses in the mSOFC components to avoid rapid degradation.

Model Explanation

This study develops a 3D full stack model and a 3D single tube model to investigate warm idle operation condition and opportunities of optimization of fuel flow rates to improve transient response and mitigate degradation using COMSOL. The 3D full stack model provides realistic temperature distributions for a single tube near the heat exchanger shield of a commercial SOFC product and has been compared with experimentally measured temperatures near the reactor and burner. The simulated temperature distribution from the stack is imposed on the single tube model to study stress distribution and electrochemistry. The full stack model has simplified tube geometry, and is sufficiently accurate to estimate for the temperature distribution. The single tube model includes the detailed layered electrode structure to predict phenomena such as delamination. From the post-mortem analysis of actual stacks, it is suspected that the outer tubes of the stack suffers the highest stress. The inlet and outlet temperature boundary conditions of the single tube are imposed using the value found from simulation of the 3D full-stack model. The internal heat generations and exothermic heat loss are used by the single tube model. Inside the single tube model, laminar flow module with porous media is used to simulate reaction flows of fuel mixture and air. Mass transport is also considered in this model to capture the concentration of reactants and the density of the fluid.

A single mSOFC tube has four cylindrical layers: anode support layer, anode functional layer, electrolyte, and cathode. Both anode support layer and anode functional layer are made of Ni-YSZ (Yttria-stabilized zirconia), but they have different composition ratio. The anode functional layer has high YSZ volume ratio. The electrolyte layer is made of YSZ and the cathode layer is Lanthanum Strontium Cobalt Ferrite (LSCF). In 3D single tube model coordination, the fuel mixture flow from the bottom of the tubular SOFC into the combustor, which is fixed at the top of the tube. Air-fuel mixture flows into a porous catalytic partial oxidation (CPOX) region inside the tube, where the fuel oxidizes. The reactant gases of electrochemical reactions, mainly H_2 and CO, are formed at chemical equilibrium at the local CPOX temperature.

The bottom of the tube is surrounded by a fixed insulator. The cathode surface is exposed to the air flow, which enters near the inlet of the anode above the insulation and exits at the porous combustor. In the solid stress module, side surfaces of the combustor and the insulator are fixed in the out-of-plane direction, but free of traction. Moreover, the top surface of the combustor is also a fixed boundary. Temperature distribution is calculated from the heat transfer module that includes surface-to-surface radiation and coupled to the solid mechanics module to obtain thermal stresses. The mSOFC is manufactured at 1473 K and 1373 K [1,7], so the stress-free temperature is above the normal operating temperature of the materials. The combustor and the insulator on the other hand are cold fabricated. Besides the thermal expansion, the volume elastic expansion of Ni- NiO redox cycling is also considered. Stathis et al. observed an increase in expansion with oxidation temperature in air, from 0.27% to 0.54% at 650 and 800 ^{o}C, respectively [8]. This redox cycling also contributes to fatigue of the materials and crack propagation of the cell layers, which leads to device failure.

Preliminary Results

Figure 1 shows two sensitivity studies of the stress concentration. In order to understand the performance of the solid mechanics simulation, plots of radial and axial stress distribution are shown. As expected, from Figure 1.b), the stress is concentrated at the two end of the active region of the tube due to the structure and relative positions to the heat sources. The lower end of the active region is close to the CPOX region, and heat generation of CPOX reactions cause increased stress. The stress distribution is almost linear across the active SOFC region. Once it reaches to the end of the active region, the stress increases due to the structure design and the maximum stress concentrates around the end region. As the mean temperature increases, the stress curves shift upward uniformly. On Figure 1.a), from radial perspective, the anode function layer suffers the lowest stress since it can expands freely inward.

The stress discontinuity between layers is caused by the mismatch of thermal expansion coefficient between layers, (the radial temperature distribution across the tube is negligible). Both the anode and cathode layers have higher thermal expansion than the electrolyte. The lower thermal expansion of the electrolyte layer causes higher stress concentration at the cathode interface, which verifies the experimental results from teardown analysis where the cathode layer showed cracking. The results also agree with the similar studies in literature [1,8]. As the mean temperature of shell rises, the stress curves also shift upward linearly and the maximum stress values are linearly related to the mean shell temperature.

We are currently working on the transients during startup and shutdown cycling and a simplified state model to optimize the flow control to mitigate the thermal and Ni oxidation/reduction stresses and improve the lifetime of the stack as well as to alleviate the carbon formation at low temperatures.

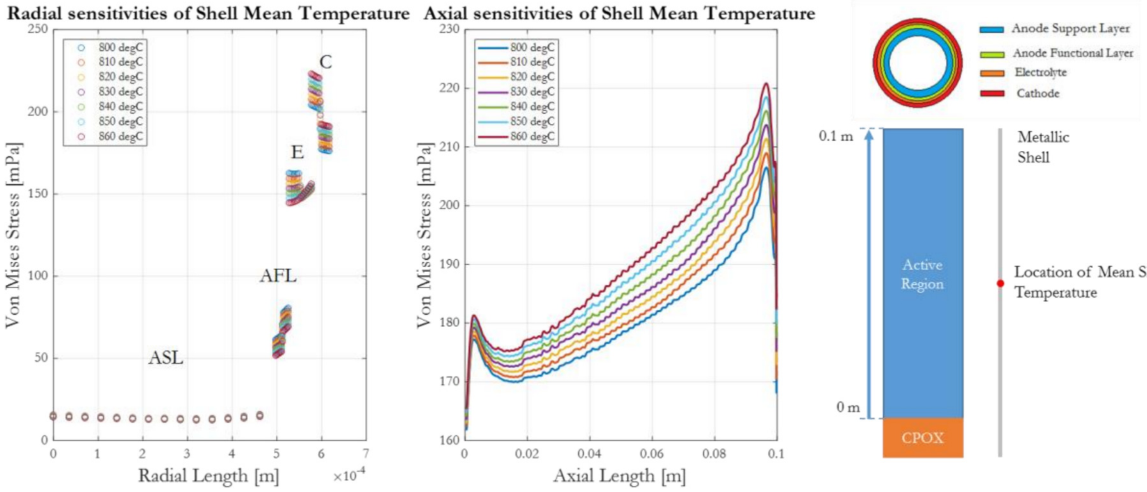

Figure 1. Sensitivities of Single Tube Stress Distribution a) Radial Stress Distribution at the top end of the active region. (ASL: Anode Support Layer, AFL: Anode Functional Layer, E: Electrolyte, C: Cathode) b) Axial Stress Distribution along the active region of the tube. C) Top and side views of active region of SOFC

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