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Grant Hawkes
James O'Brien
Carl Stoots
Brian Hawkes

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3D CFD MODEL OF A MULTI-CELL HIGH TEMPERATURE ELECTROLYSIS STACK

Grant Hawkes, James O'Brien, Carl Stoots, Brian Hawkes
Idaho National Laboratory, Idaho Falls, Idaho

Abstract

A three-dimensional computational fluid dynamics (CFD) electrochemical model has been created to model high-temperature electrolysis stack performance and steam electrolysis in the Idaho National Laboratory Integrated Lab Scale (ILS) experiment. The model is made of 60 planar cells stacked on top of each other operated as Solid Oxide Electrolysis Cells (SOEC). Details of the model geometry are specific to a stack that was fabricated by Ceramatec, Inc[1]. and tested at the Idaho National Laboratory. Inlet and outlet plenum flow and distribution are considered. Mass, momentum, energy, and species conservation and transport are provided via the core features of the commercial CFD code FLUENT[2]. A solid-oxide fuel cell (SOFC) model adds the electrochemical reactions and loss mechanisms and computation of the electric field throughout the cell. The FLUENT SOFC user-defined subroutine was modified for this work to allow for operation in the SOEC mode. Model results provide detailed profiles of temperature, Nernst potential, operating potential, activation over-potential, anode-side gas composition, cathode-side gas composition, current density and hydrogen production over a range of stack operating conditions. Variations in flow distribution, and species concentration are discussed. End effects of flow and per-cell voltage are also considered.

Introduction

A research program is under way at the Idaho National Laboratory (INL) to simultaneously address the research and scale-up issues associated with the implementation of planar solid-oxide electrolysis cell technology for hydrogen production from steam. The research program includes an experimental program aimed at performance characterization of electrolysis cells and stacks. Results of some multi-cell tests have been documented in several recent papers [1], [2]. This paper reports the first plenum study of a 60 cell stack when modeling a planar solid oxide electrolysis cells (SOEC) with the FLUENT code and SOFC module [3]. This code was used for detailed SOEC modeling. Fluent Inc. was funded by the US Department of Energy National Energy Technology Laboratory (DOE-NETL) to develop a solid-oxide fuel cell (SOFC) module for coupling to the core mass, momentum, energy, and species conservation and transport features of the FLUENT CFD code. The SOFC module adds the electrochemical reactions and loss mechanisms and computation of the electric field throughout the cell. The FLUENT SOFC user-defined subroutine was modified for this work to allow for operation in the SOEC mode. Model results provide detailed profiles of temperature, Nernst potential, operating potential, anode-side gas composition, cathode-side gas composition, current

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[1,2] References herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government, any agency thereof, or any company affiliated with the Idaho National Laboratory

density and hydrogen production over a range of stack operating conditions. Reference [4] has details of the FLUENT code and numerical model. Results of the numerical model are shown in this paper.

Numerical Model

The numerical model developed for this paper was based on the geometry of a 60 cell stack fabricated by Ceramatec, Inc. and tested at the INL. A depiction of four 60-cell stacks comprising an ILS module is shown in Figure 1. The stack has a per-cell active area of 64 cm^2. It is designed to operate in cross flow, with the steam/hydrogen gas mixture entering the inlet manifold on the right/front in the depiction, and exiting through the outlet manifold located in the center. Air flow enters at the other center manifold (not visible in Fig. 1) and exits at the front/left where the tabs are shown directly into the furnace. The power lead attachment tabs, integral with the upper and lower interconnect plates are also visible in the depiction. Figure 2 shows the piping for the H2/H2O inlet and outlet and air inlet. Figure 3 shows a blown up view of a single cell with its components that are scaled 10x in the z-direction.

The numerical model geometry represents a complete 60 cell stack that is ¼ of the ILS module. Symmetry boundary conditions are implemented. The numerical domain extends from the bottom of the inlet tubes to the outlet flow path of each stream. Inlet flow tubes for the H2/H2O and air side are modeled 5-in. below the inlet of the plenum. This distance allows the flow to develop.

The FLUENT SOFC module treats the electrolyte as a 2-D planar element. Therefore the electrolyte in the model has geometrical thickness of zero. The electrolyte has a thickness of 0.14 mm. This thickness was apportioned to the separator plates so as to keep the total stack height correct. On either side of the electrolyte are the electrodes that are created with 3-D elements. Therefore, the electrolyte/electrode assembly in the model is only as thick as the two electrodes.

Approximately 1.5 million elements are included in this model. Figure 4 shows the top view of

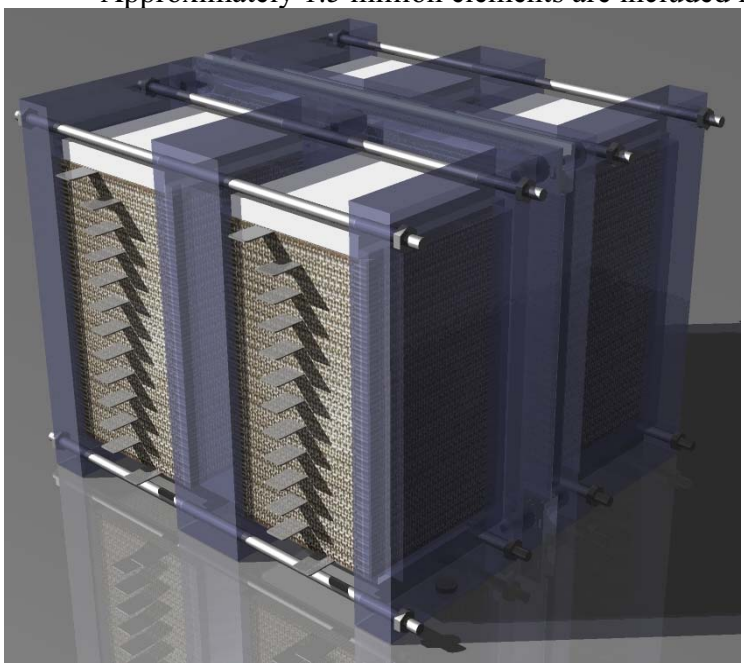


Figure 1. Depiction of ILS module with four 60-cell stacks. Green = air inlet, pink = H2/H2O inlet, orange = H2 outlet.

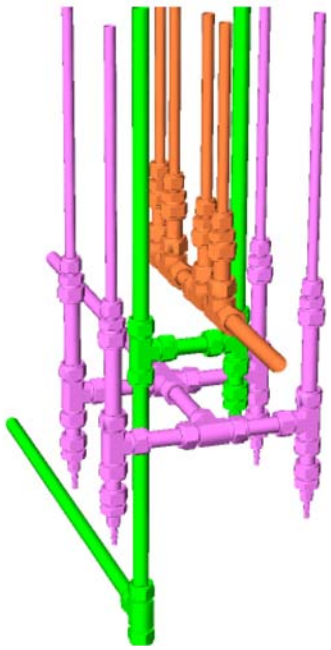


Figure 2. Inlet and outlet piping maze.

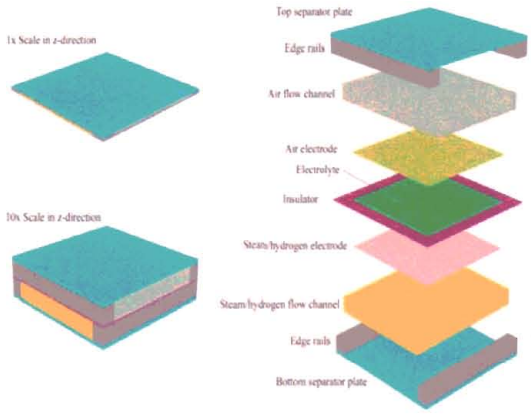


Figure 3. Component description for a single cell.

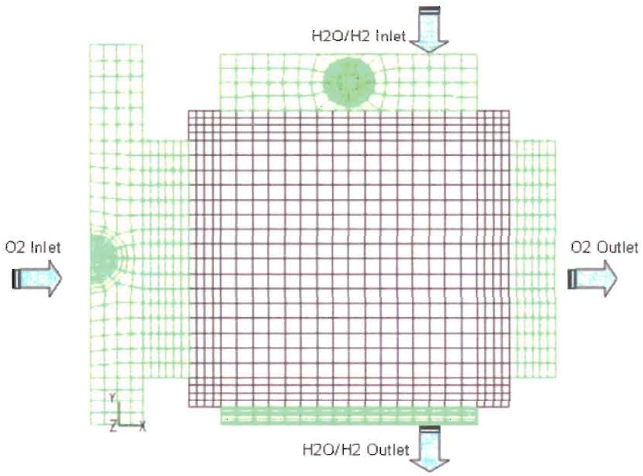


Figure 4. Mesh used at each cross section in z-dir.

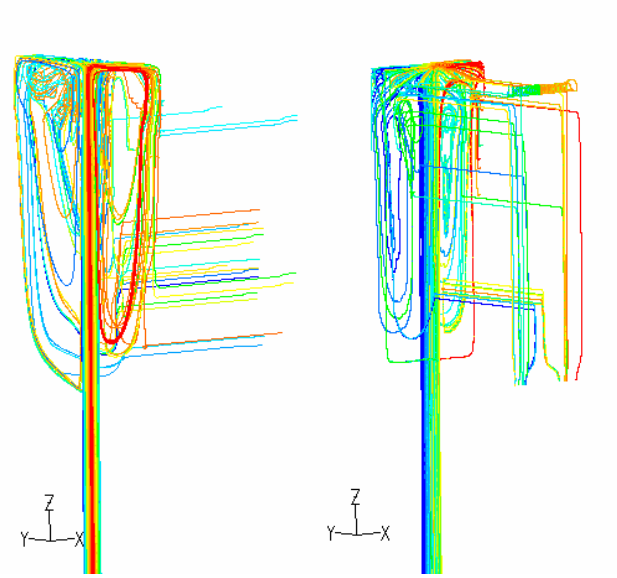
the grid used. This grid was used at each level throughout the entire height of the model. The numerical grid used in this study included 4 elements each in the flow inlet and outlet regions, and 16 x 16 in the active cell area in the X and Y directions. Each flow channel (current collector) has 6 elements across the flow channel. Single cell numerical models with these numbers of cells give identical results to twice as many, meaning that the model is grid converged in the cell area. More research needs to be done on the mesh in the inlet and outlet plenum areas.

All external surfaces are considered to be adiabatic. Details of the core mass, momentum, energy, and species conservation and transport features of FLUENT are documented in detail in the FLUENT user manual from Fluent Inc. Details of the electrochemical reactions, loss mechanisms, electric field computation, and electrode porous media constitutive relations are documented by the SOFC module in the FLUENT documentation. This reference also documents the treatment of species and energy sources and sinks arising from the electrochemistry at the electrode-electrolyte interfaces.

Mass flow rates, compositions, and other parameters were taken from the base case of Reference [5].

Results

Results are displayed on Figures 5 through 14. Figures 5 and 6 show the path lines of the flow for the air inlet and H2/H2O inlet at open cell voltage (OCV) respectively. Most of the flow appears to go all the way to the top of the plenum and then recirculate down the outside before entering into each cell. Shown in Figure 7 are temperature contour plots displayed on the H2 side current collector, H2/H2O inlet plenum, and air inlet plenum for open cell voltage (OCV), 60 V, 77.2 V, and 80 V. These values correspond to 1.0, 1.28667, and 1.333 V/cell respectively. Since the inlet temperature is at 1073 K, the thermal neutral voltage is 1.28667 V/cell. The scale for each figure goes from the minimum to the maximum for each particular model. The second figure is dominated by the endothermic reaction and shows temperatures well below the inlet conditions, while the third figure has a mean outlet gas temperature exactly equal to the inlet temperature of 1073 K. The fourth figure shows that temperatures are dominated by the Ohmic heating in the electrolyte and well above the thermal neutral condition.



Figures 5 and 6. Pathlines for O2 (left) and H2/H2O (right)

Figure 8 shows the Nernst potential on each electrolyte for the same four operating voltages. Nernst potential depends on the gas compositions and temperature. The temperature is dependent on the current density because of the endothermicity of the reaction. Figure 9 shows the current density on each electrolyte in the stack. The highest magnitude of current density and hence H2 production are the most negative. Shown in Figure 10 are the voltages at each separator plate. The colors are all the same because the scales are different for each figure. Figure 11 shows the H2 mole fraction in the H2/H2O inlet plenum, H2 current collector, and the surface on the outlet of the H2/H2O outlet plenum. For the thermal neutral case, the most H2 is produced about ¾ of the way up the stack. Shown in Figure 12 is the O2 mole fraction displayed on the O2 current collector, and air inlet plenum. The amount of O2 produced is higher near the H2/H2O inlet side. This is due to the high concentration of H2O available to be electrolyzed as shown by the Nernst potential.

Figures 13 and 14 show the per cell mass flow rate exiting each cell for the H2/H2O and O2 side respectively. The OCV shows the flow through the stack with no current. The flows all have the highest flow near the bottom cells. Figure 14 shows the O2 production rate is increasing with the increase in voltage and hence current. The flow through the O2 cells during OCV is quite constant.

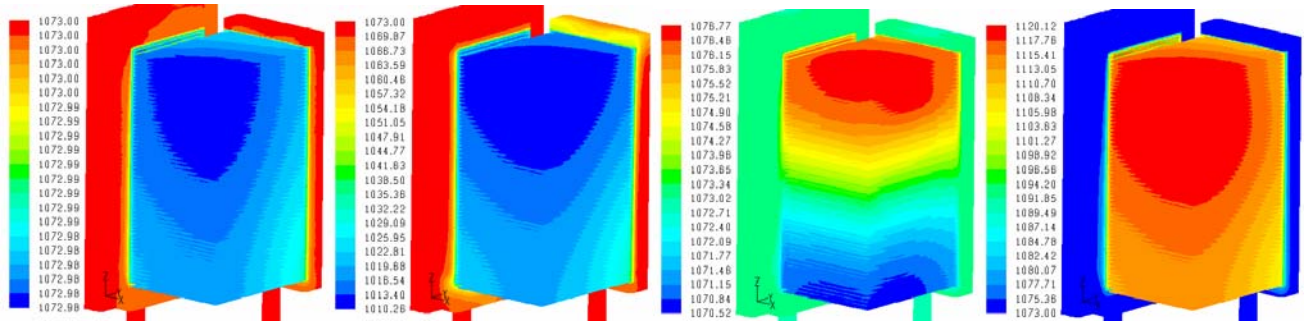


Figure 7. Temperature (K) contours for OCV, 60V, 77.2V, and 80V.

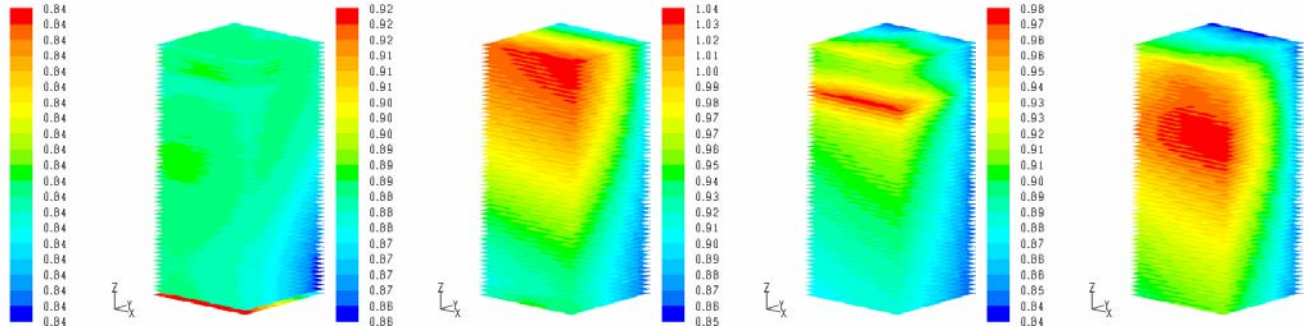


Figure 8. Nernst potential (V) for OCV, 60V, 77.2V, and 80V.

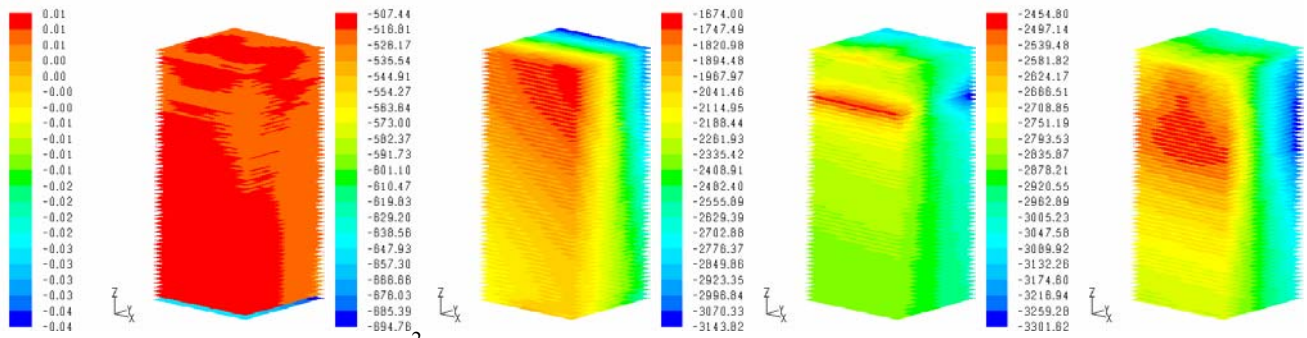


Figure 9. Current density (A/m^2) for OCV, 60V, 77.2V, and 80V.

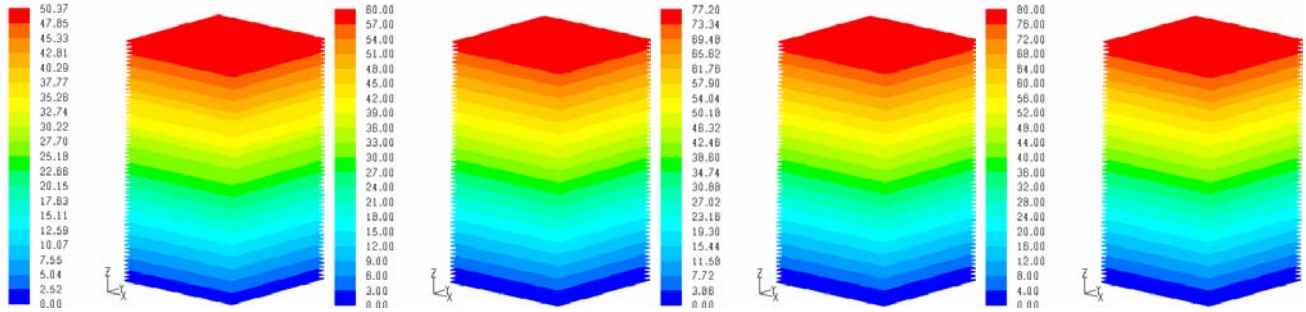


Figure 10. Operating voltage (V) for OCV, 60V, 77.2V, and 80V.

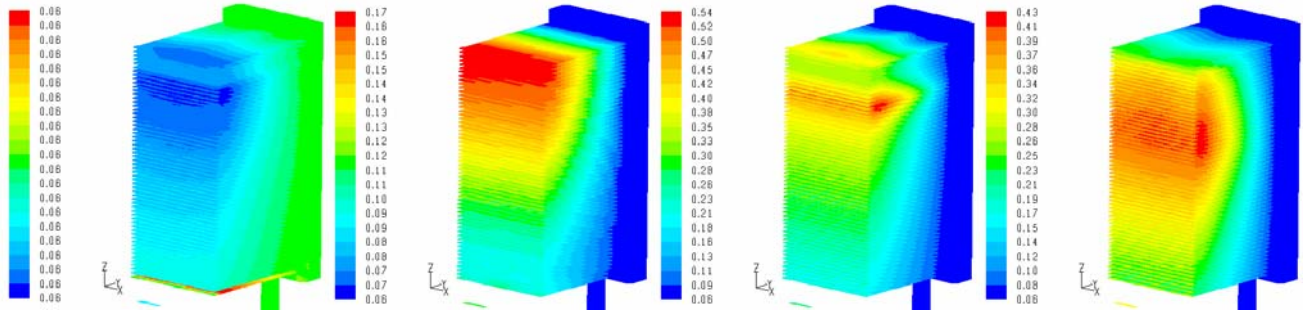


Figure 11. H2 mole fraction for OCV, 60V, 77.2V, and 80V.

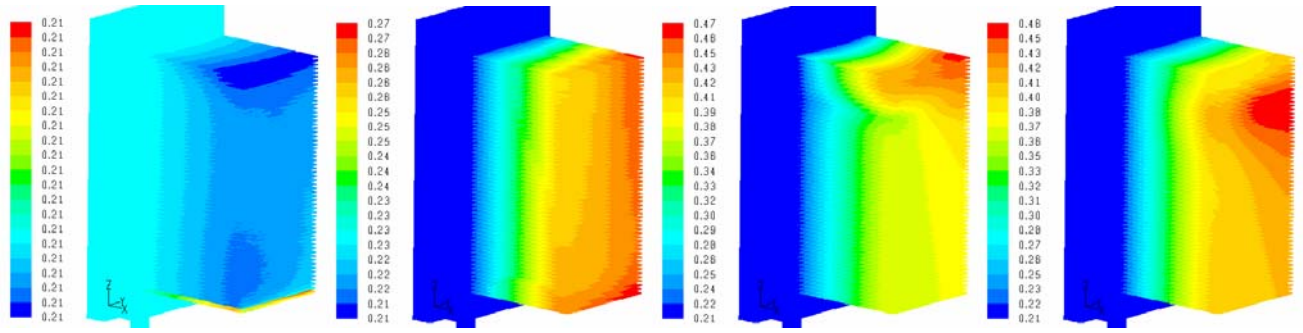
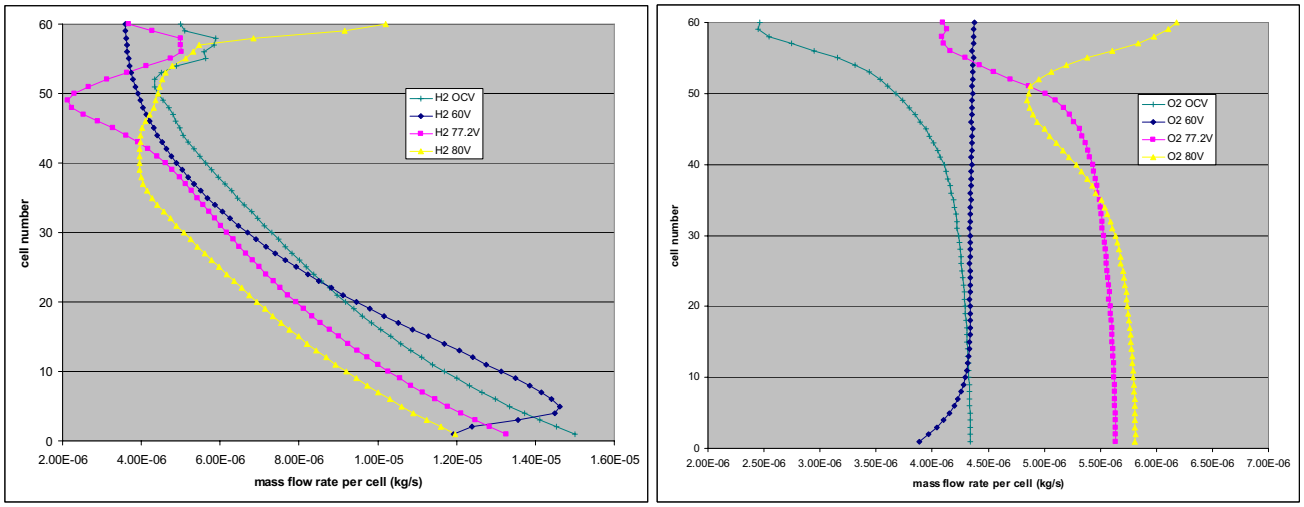


Figure 12. O2 mole fraction for OCV, 60V, 77.2V, and 80V.



Figures 13 and 14. Mass flow rate exiting per cell for H2 and O2 respectively.

Conclusions

A three-dimensional computational fluid dynamics (CFD) model has been created to model high-temperature steam electrolysis in a planar solid oxide electrolysis cell (SOEC) stack. Effects of the variation of input parameters are shown for this stack and model. The model represents 60-cell stack that represents a ¼ of an ILS module. Details of the model geometry are specific to a stack that was fabricated by Ceramatec, Inc. and tested at the Idaho National Laboratory. Mass, momentum, energy, and species conservation and transport are provided via the core features of the commercial CFD code FLUENT. A solid-oxide fuel cell (SOFC) model adds the electrochemical reactions and loss mechanisms and computation of the electric field throughout the cell. The FLUENT SOFC user-defined subroutine was modified for this work to allow for operation in the SOEC mode. Model results provide detailed profiles of temperature, Nernst potential, operating potential, anode-side gas composition, cathode-side gas composition, current density and hydrogen production over a range of stack operating conditions. Inlet and outlet plenums are included in the model of this stack. Plenum flow characteristics with recirculation were observed. Contour plots of local electrolyte temperature, current density, and Nernst potential indicated the effects of heat transfer, reaction cooling/heating, and change in local gas composition.

Acknowledgements

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References

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[4] G. L. Hawkes, J. E. O'Brien, C. M. Stoots, J. S. Herring, "CFD Model of a Planar Solid Oxide Electrolysis Cell for Hydrogen Production from Nuclear Energy," *Nuclear Technology*, Vol. 158, pp. 132 - 144, May, 2007.

[5] G. L. Hawkes, R. W. Jones, "CFD Model of a Planar Solid Oxide Electrolysis Cell: Base Case and Variations," 2007 ASME-JSME Thermal Engineering Conference and Summer Heat Transfer Conference, July 8 – 12, 2007, Vancouver, BC, Canada.