SOFC-MP

Modeling Tools for Solid Oxide Fuel Cell Stacks

Kevin Lai, Brian J. Koeppel, Moe A. Khaleel

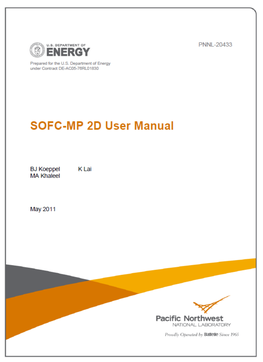
Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

Objective

Develop modeling tools to evaluate the tightly coupled multi-physics of solid oxide fuel cell (SOFC) stacks and enable SOFC manufacturers to numerically test the effects of stack design, materials, and operation on overall performance and mechanical reliability.

Technical Approach

- SOFC-MP is a simulation tool developed at PNNL to evaluate the tightly coupled multi-physical phenomena in SOFCs. The purpose of the tool is to allow SOFC manufacturers to numerically test changes in planar stack design to meet DOE technical targets.
- The SOFC-MP software tool consists of two modules:
  - 2D Module: This model is designed for computational efficiency to enable rapid engineering evaluations for operation of tall symmetric stacks. It can quickly compute distributions for the current density, voltage, temperature, and species composition in tall stacks with co-flow or counter-flow orientations.
  - 3D Module: This model is designed to compute the thermal-mechanical stresses of fully detailed stacks during operation. It provides not only the same physical quantities as the 2D model (i.e., current density, voltage, temperature, and species composition), but also the stresses due to mechanical and thermal loads.



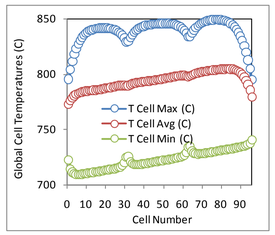
Recent Accomplishments

- A detailed user manual for the 2D SOFC-MP module describing installation, model creation, solution, and results evaluation was completed.
- An installation CD containing the 2D SOFC-MP module, demonstration cases, and a post-processing spreadsheet tool was completed.
- The 2D module was successfully benchmarked against single and multi-cell literature cases.
- The 2D module was used to perform a parameteric study on the effects of design and operation on temperature uniformity of a tall 25kW stack.
- For the 3D module, a roadmap was developed for transfer of the model and solution technology to a flexible framework for wider usage with other finite element analysis (FEA) packages.

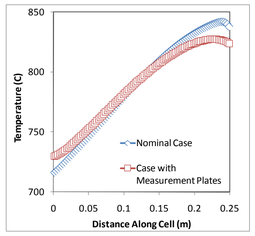
Rich Features in 2D Model

- The 2D model is able to simulate different flow orientations, cell count, cell size, boundary conditions, fuels, user-defined electrochemistry and reforming.

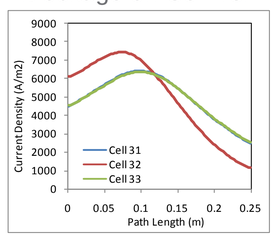
Effect of Instrumented Measurement Plates



Cell ΔT Error from Measurement Plate



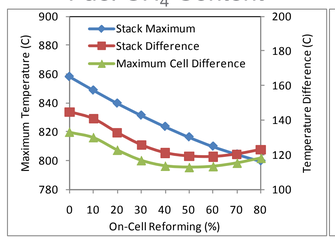
Effect of 25% Fuel Blockage on Cell #32



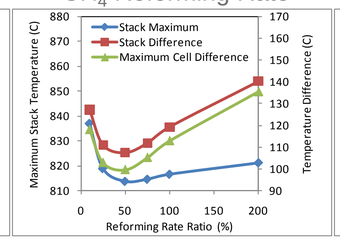
Parametric Study Using 2D Model

- Effect of design changes on temperature uniformity of 96-cell 25kW stack:
  - Optimal CH_4 fuel composition and reforming rate predicted for co-flow design.
  - Thinner interconnects reduce cost, but lower thermal conduction increases ΔT.

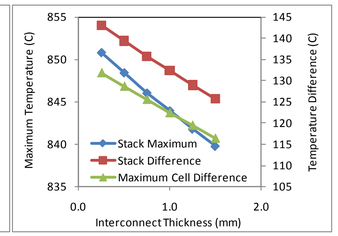
Fuel CH_4 Content



CH_4 Reforming Rate

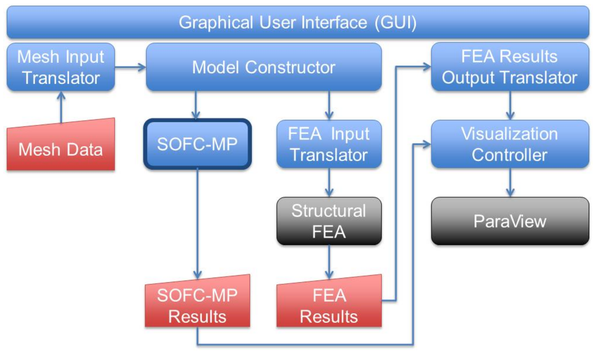


Interconnect Thickness



Flexible Framework for 3D Model

- The existing 3D model is currently tightly integrated with the commercial FEA code MSC Marc for model creation, mechanical solution, and post-processing.
- To increase usage of the tool by eliminating licensing costs, the code will be transferred to a more generic framework which can interface with various commercial FEA packages and uses open source ParaView for post-processing.



Future Work

- Add functionality to 2D SOFC-MP for user definition and control of state variables:
  - Simulate pseudo-transient degradation such as thermal distribution change due to oxide scale growth on the interconnect.
  - Provide multi-scale coupling with the distributed electrochemistry (DEC) model.
- Complete generic framework for the 3D modeling package .

Publications

- C Lai, BJ Koeppel, M. Khaleel etc. “A Quasi-Two-Dimensional Electrochemistry Modeling Tool for Planar Solid Oxide Fuel Cell Stacks”, J. Power Source, 196(6), 2011.
- BJ Koeppel, C Lai, MA Khaleel, “Effect of Geometry and Operating Parameters on SOFC Stack Temperature Uniformity,” to be presented at 9th Fuel Cell Science, Engineering, and Technology Conference, Aug 7-10, 2011, Washington, DC.
- BJ Koeppel, C Lai, MA Khaleel, “SOFC-MP 2D User manual,” PNNL-20433.

Acknowledgement

This work was funded as part of the Solid-State Energy Conversion Alliance Core Technology Program by the U.S. Department of Energy’s National Energy Technology Laboratory.

For more information, please contact:

Kevin Lai, Brian J. Koeppel, Moe A. Khaleel
Pacific Northwest National Laboratory
Richland, WA 99352
Canhai.Lai@pnnl.gov