SOFC-MP

Modeling Tools for Solid Oxide Fuel Cell Stacks

Kevin Lai, Brian J. Koeppel, Khushbu Agarwal, Wenxiao Pan, Moe A. Khaleel

Pacific Northwest NATIONAL LABORATORY

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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 operating state on overall performance and mechanical reliability.

Technical Approach

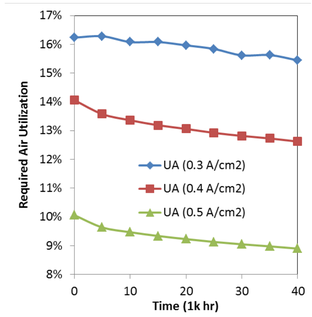
- SOFC-MP is a simulation tool developed at PNNL to evaluate the flow, thermal, and electrochemical phenomena in SOFCs. Its purpose is to aid the experiments and design efforts of SOFC manufacturers by enabling them to numerically assess the impact of design changes on performance.
- The SOFC-MP software tool suite consists of four integrated modules:
  - 2D Module: This module 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 module 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 module (i.e., current density, voltage, temperature, and species composition), but also the component stresses due to mechanical and thermal loads on the stack.
  - User Interface: The user-friendly GUI invokes 2D and 3D simulations, and handles all pre- and post-processing needed for the simulations.
  - SOFC-MP ROM: This reduced order model (ROM) uses response surface analysis to provide a high fidelity, robust, and efficient way to calculate stack performance data when input parameters are varied.

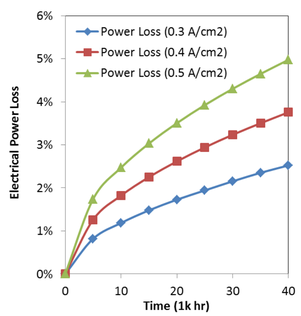
Recent Accomplishments

- Degradation modeling: User definition and calculation of state variables has been added to the SOFC-MP 2D module. This added feature can simulate pseudo-transient degradation by general mechanisms (e.g., temperature state change due to oxide scale growth on the interconnect).
- Reduced Order Modeling (ROM): A new software tool SOFC-MP ROM Builder was created to efficiently provide robust and high fidelity results for system-level models based on the established 2D tool, though the ROM framework is flexible such that it can take results from any user model or experiment. Advanced mathematics for ROM efficiency and accuracy have been evaluated and implemented in the software for SOFC analysis.
- User Interface: Added user-friendly GUI for 2D and 3D simulations.

Improved 2D Module: Degradation Simulation

- A multi-step solution framework was implemented within SOFC-MP 2D to simulate evolution of cell electrochemical parameters and their effects on stack performance.

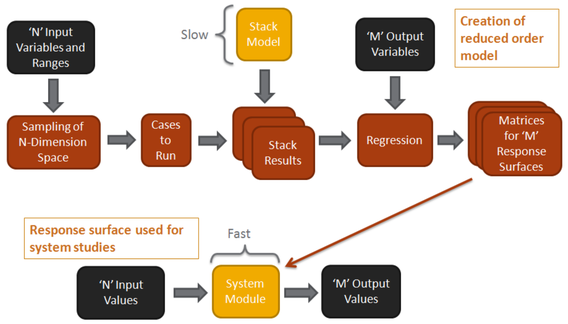


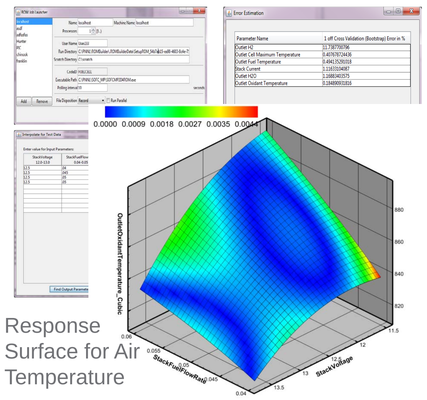


Predicted air utilization required to maintain 850ºC maximum cell temperature and associated power loss for a 96-cell 25kW stack due to interconnect scale growth

Reduced Order Modeling Framework and Tool

- The SOFC-MP ROM Builder tool uses results from detailed stack analyses with response surface analysis to automatically create a ROM that can efficiently provide robust and high fidelity results suitable for modeling of fuel cell power plant systems.

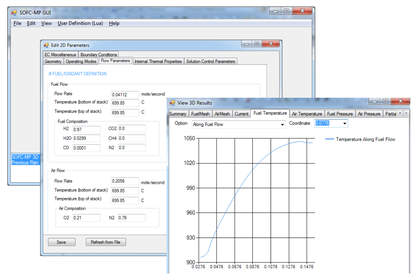




Response Surface for Air Temperature

Flexible User Interface for SOFC-MP Tools

- To increase usage of the SOFC-MP tools by eliminating expensive licensing costs, the 3D code is being transferred to a more generic framework which can interface with various commercial FEA packages and uses open source ParaView for post-processing.
- The suite of codes will then be combined under a single common user interface for convenience.



Future Work

- Demonstrate and release the SOFC-MP ROM package.
  - Demonstrate ROM creation and usage for fuel cell based power plant configurations.
- Determine the influence of high water conditions on long term stack operating performance.
- Complete stack benchmarking comparisons for the 3D modeling package with experimentally-measured data.
- Release SOFC-MP software tool suite which consists of 2D module, 3D module, GUI, and SOFC-MP ROM.

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For more information, please contact:

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

Pacific Northwest National Laboratory

Richland, WA 99352

Kevin.Lai@pnnl.gov