

## Efficient Numerical Investigation of Fuel Cell Performance Under Various Conditions

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There have been extensive efforts devoted to proton exchange membrane (PEM) fuel cell modeling and simulation to study the fuel cell performance under various conditions. The research spans from atomic and quantum level way up to the fuel cell system and even to the fuel cell power train. We tend to categorize the fuel cell modeling and simulation activities into four levels: micro level, single cell level, stack level and system level. The current study will focus on single cell level, however, with the future integration with other levels in mind.

The multi-resolution fuel cell simulation approach [1,2] is employed in this study. For membrane, a full 3D modeling is employed due to the fact that transport present in the membrane includes both convection and diffusion in all directions. Catalyst layer is modeled as 1D+2D, that is, at each location of the fuel cell plate, the governing equations are integrated only in the direction perpendicular to the fuel cell plate. The diffusion layer is modeled as full 3D flow due to the domination of diffusion process present. A quasi-1D method with high numerical efficiency and reasonable accuracy is employed to model gas flow channels. In addition, both anode and cathode activation over-potential are computed according to the specified cell potential and reversible fuel cell potential.

All these models are dynamically integrated based on Loci system [3], which is developed at Mississippi State University. The Loci system is an application framework that seeks to reduce the complexity of assembling large-scale finite-difference, finite-volume, or finite-element applications.

An industrial size single cell has been used to demonstrate the efficient simulation capabilities. The flow channel patterns evaluated will include serpentine, parallel and combined serpentine-parallel patterns, and different flow patterns can be used for the cathode and anode sides. A parameter sensitivity study through the integrated fuel cell simulation framework will also be presented in this paper to investigate the effect of various operating, geometric and material parameters on the performance of PEM fuel cells.

### References

1. Wu, J. and Liu, Q., 2003 "Integrated Multi-resolution Fuel Cell Simulation," in the *204<sup>th</sup> ECS Proceedings of Power Sources for Transportation Applications*, Landgrebe, A.R., ed., in press.
2. Wu, J. and Liu, Q., 2004 "Simulation Aided PEM Fuel Cell Design and Performance Evaluation," First International Conference on Fuel Cell Development and Deployment, Storrs, CT.
3. E. A. Luke, "A rule-based specification system for computational fluid dynamics," Ph.D. thesis, Mississippi State University, 1999.

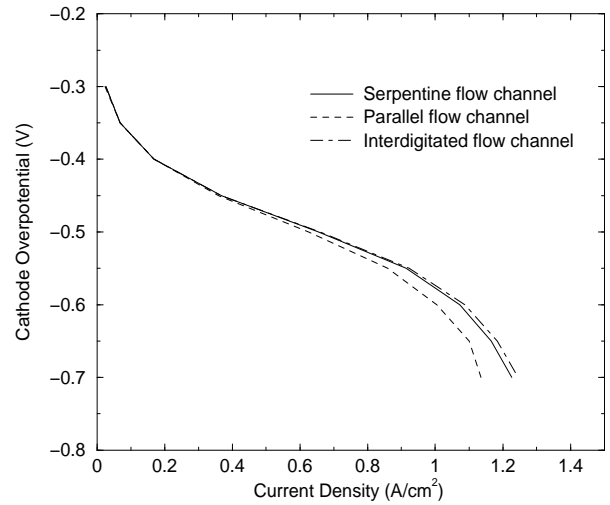


Figure 1. Comparisons of the polarization curves for various channels.

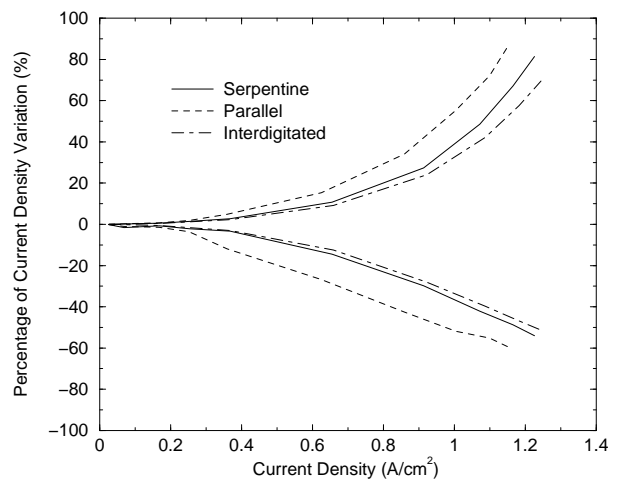


Figure 2. Comparisons of the current density variation as a percentage of the respective average current density for various channels.