

**PPDO-132**  
**Multi-scale Modeling and Optimization of PEM Fuel Cells**

**Myung S. Jhon**

Professor, Chemical Engineering Department, Carnegie Mellon University,  
Pittsburgh, PA

**Lorenz T. Biegler**

Professor, Chemical Engineering Department, Carnegie Mellon University,  
Pittsburgh, PA

**Abstract**

Because of the high efficiency and zero or ultra-low emissions, fuel cell (FC) technology promises to provide alternatives for the internal combustion engine and hybrid power generation. Proton electrolyte membrane fuel cells (PEMFCs) recently attracted attention due to their high power density, low temperature operation, and nearly instantaneous recharging. There are two types of PEMFCs, i.e., H<sub>2</sub> PEMFC and direct methanol fuel cells (DMFCs), both of which utilize PEM to transfer proton and they are the primary focus of our proposed work.

Our objective is to construct simulation and optimization tools for FCs. We adopt a multi-scale systems approach, which includes micro/nano-scale (e.g., interfacial region of reactant, electrolyte, and membrane-electrode assembly), meso-scale (e.g., fuel cell units), and macro-scale (e.g., power generation system). Optimization will be employed at all scales. In our previous work, we performed successful optimization both in the meso- and macro-scale. In this proposal, our focus will be on the micro/nano-scale, i.e., the study of the property and structure relationships for the PEM, via Monte Carlo (MC) and molecular dynamics (MD) simulation as our primary tools. This PEM model will not only reveal the physics of the PEM, but can also be “up-cast” and incorporated into the meso-scale model, which can be used for optimization study. Sensitivity analysis and nonlinear programming (NLP) techniques will be applied for the numerical analysis and optimization. Our preliminary results on the DMFC and H<sub>2</sub> PEMFC systems have shown great promise in the application of optimization techniques in the FC area. Further improvements in both the physical and numerical aspects can be expected from current study to provide guidelines for the production and operation of FCs to achieve their commercialization.