Large-Scale PEM Fuel Cell Modeling by Parallel Computation

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Polymer electrolyte membrane (PEM) fuel cells are considered as promising alternative power plants for transportation because of their high efficiency, high power density, low emissions, low operation temperature, and low noise. In the past decade, significant improvements have been achieved in PEM fuel cell technology, including improved membrane-electrode assembly (MEA) and lowered platinum catalyst loading. As in many engineering fields, numerical modeling and simulation become important tools for enhancing physical understanding and improving engineering design of PEM fuel cells. Current development in PEM fuel cell modeling is in the direction of applying computational fluid dynamics (CFD) to solve the complete set of transport equations governing mass, momentum, species, energy, and charge conservation.

In this paper, an electrochemical-transport fully coupled PEM fuel cell model is implemented into a commercial CFD package, Star-CD, based on its user coding capability. All seven regions of a PEM fuel cell, namely anode gas channel, anode diffusion layer, anode catalyst layer, membrane, cathode catalyst layer, cathode diffusion layer, and cathode gas channel, are considered in the current numerical model. Large-scale numerical modeling of a PEM fuel cell with 5-channel serpentine flow-field, 1 million total computational cells, is carried out by parallel computation using our in-house Linux PC cluster. Since advanced numerical algorithms have been employed in the current numerical model, extremely efficient calculations are achieved, requiring roughly 300 iterations for a typical case-run. Model validation is shown in Fig. 1, illustrating excellent agreement between numerical and experimental results. Figure 2 shows the computational speed-up of the PEM fuel cell simulation using our PC cluster, demonstrating more than seven times improvement in computation time using 10 CPUs. Figure 3 shows the polarization and power curves for a PEM fuel cell with Nafion 111 membrane, operating at 80 ^{o}C and 2 atm with fully humidified gas streams in both anode and cathode inlets. Figure 4 illustrates the current density variations in membrane under each channel, indicating higher local current density within the U-turn regions. The explanation for this phenomenon is that oxygen is better mixed within U-turn regions in cathode gas channels and, therefore, results in higher oxygen concentration and faster electrochemical kinetics in the cathode catalyst layer underneath. Extensive calculations reported in this work prove that the parallelized numerical model is accurate, efficient, and capable of handling large and complicated flow fields, as well as detailed electrochemical and transport phenomena, in a PEM fuel cell.

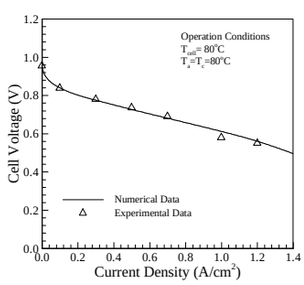

Fig. 1. Model validation

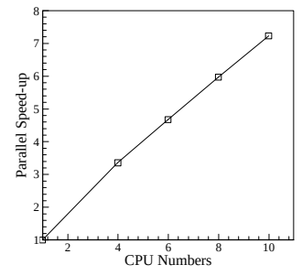

Fig. 2. Parallel performance

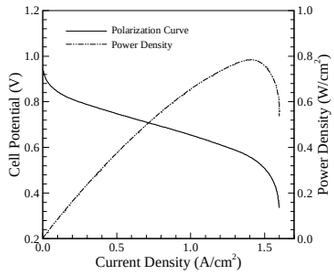

Fig. 3. Polarization and power density curves

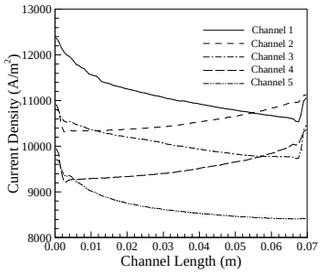

Fig. 4. Current density variations under gas channels