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Using an ILU/Deflation Preconditioner for Simulation of a PEM Fuel Cell Cathode Catalyst Layer

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Abstract. Numerical aspects of a pore scale model are investigated for the simulation of catalyst layers of polymer electrolyte membrane fuel cells. Coupled heat, mass and charged species transport together with reaction kinetics are taken into account using parallelized finite volume simulations for a range of nanostructured, computationally reconstructed catalyst layer samples. The effectiveness of implementing deflation as a second stage preconditioner generally improves convergence and results in better convergence behavior than more sophisticated first stage pre-conditioners. This behavior is attributed to the fact that the two stage preconditioner updates the preconditioning matrix at every GMRES restart, reducing the stalling effects that are commonly observed in restarted GMRES when a single stage preconditioner is used. In addition, the effectiveness of the deflation preconditioner is independent of the number of processors, whereas the localized block ILU preconditioner deteriorates in quality as the number of processors is increased. The total number of GMRES search directions required for convergence varies considerably depending on the preconditioner, but also depends on the catalyst layer microstructure, with low porosity microstructures requiring a smaller number of iterations. The improved model and numerical solution strategy should allow simulations for larger computational domains and improve the reliability of the predicted transport parameters. The preconditioning strategies presented in the paper are scalable and should prove effective for massively parallel simulations of other problems involving nonlinear equations.

AMS subject classifications: 65F08, 65F10, 65F15, 65F50

Key words: Deflation, PEM fuel cell, catalyst layer, pore scale model, porous media, preconditioner.

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1 Introduction

Polymer Electrolyte Membrane (PEM) fuel cells have been the focus of intense research and development in the last decade due to their high energy conversion efficiency, low to zero emissions, and suitability for a broad range of applications from transportation to portable electronic devices. A PEM fuel cell is composed of a number of different layers as shown in Fig. 1. On each side of the fuel cell are flow channels, through which oxygen and hydrogen flow. The hydrogen and oxygen diffuse through a diffusion layer to the anode and cathode catalyst layers respectively. At the anode catalyst layer, hydrogen reacts to produce protons and electrons. The protons travel through the polymer membrane to the cathode catalyst layer, while the electrons go through an external circuit to do useful work. The electrons, protons and oxygen electrochemically react in the cathode catalyst layer to produce water.

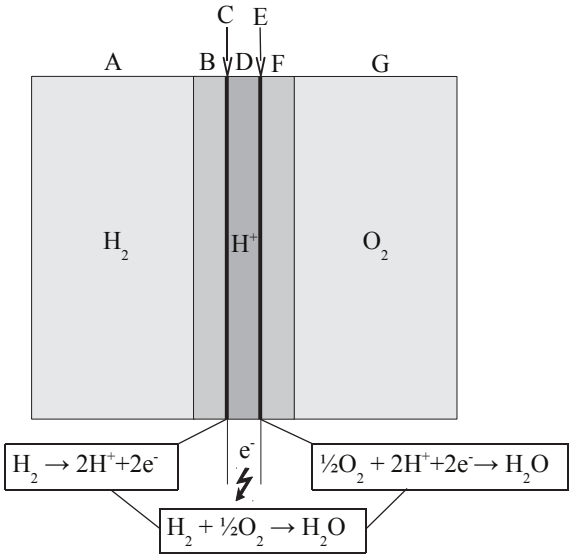

Figure 1: Simplified Schematic of PEM fuel cell operation and components: A. Anode flow channel. B. Anode gas diffusion layer. C. Anode catalyst layer. D. Polymer electrolyte membrane. E. Cathode catalyst layer. F. Cathode gas diffusion layer. G. Cathode flow channel

The operation of a PEM fuel cell relies on an array of coupled transport phenomena, including the supply of reactants, reaction kinetics, transport of ions and electrons, and removal of by-product heat and water [1]. The transport and rate limitations associated with these processes result in irreversibilities that appear as voltage losses. Many of these losses occur at the cathode catalyst layer, where the energy needed to initiate electrochemical reactions (activation polarization) is quite high [2]. A PEM fuel cell catalyst layer is a nanostructured medium composed of four distinct phases: pores which allow for reactant gas diffusion, an ionomer membrane which allows for proton conduction, carbon-black particles which allow for electron conduction, and platinum nanoparticles