

TUESDAY, AUGUST 23, 2005, P.M.

SESSION 23B: INTERNATIONAL SYMPOSIUM ON FUEL CELL AND HYDROGEN TECHNOLOGIES

MODELLING III

Sponsor(s): Materials Science and Engineering Section, The Metallurgical Society of CIM

Room: Imperial Ballroom 7

Chairmen: N. DJILALI, University of Victoria, Canada and

M. EIKERLING, Simon Fraser University, Canada

PAPER 23B.1 — 16:00

EXPLICIT SOLUTION FOR THE CATHODE CATALYST LAYERS OF PEM FUEL CELLS.

D. SONG, S. LIU, Q. WANG, NRC Institute for Fuel Cell Innovation

W.-M. YAN, Huafan University, Taipei

C.-Y. SOONG, Feng Chia University, Taiwan

In this paper, the differential equations governing the mass transport and the electrochemical reaction in a cathode catalyst layer of polymer electrolyte membrane fuel cells are solved based on the polynomial series expansion method. Explicit expressions for the polarization curve as well as for the distributions of oxygen, current density and overpotential are obtained when a quadratic, cubic or quartic polynomial is employed to approximate the oxygen concentration distribution. These kinds of explicit solutions are desirable for MEA design and diagnosis purposes. The comparison between the conventional numerical approach and the explicit solution approach proposed here shows that satisfactory accuracy can be reached by the first four terms of the polynomial series. The effect of the catalyst layer thickness on the accuracy of the obtained explicit polynomial solutions is also discussed.

PAPER 23B.2 — 16:20

EFFECTIVE DIFFUSION COEFFICIENT IN RANDOM POROUS MEDIA.

D. MU, S. LIU, C. HUANG, NRC Institute for Fuel Cell Innovation, Canada

N. DJILALI, University of Victoria, Canada

A method is presented for evaluating the effective gas diffusion coefficient of porous media. A series of random-distributed porous solids with different porosity are generated, a solution of the gas diffusion equations inside the porous media is obtained using the finite element method (FEM), and then the effective gas diffusivities are computed. The results show that there is a percolation threshold ϵ_p , and this percolation threshold decreases with an increase in the connectivity of the pore network; the relationship between the effective diffusivity and the porosity is strongly nonlinear when the porosity ϵ is less than about 0.2; and is quasi linear for higher porosities. The threshold decreases with increasing the connectivity of the pore network. A formula relating the effective diffusion coefficient with porosity is proposed.

PAPER 23B.3 — 16:40

COMPUTATIONAL FLUID DYNAMICS ANALYSIS AND FLOW VISUALIZATION OF PEMFC FLOW FIELDS.

A.M. REYES, F. TAGHIPOUR, D.P. WILKINSON, University of British Columbia, Canada

Flow field hydrodynamics of serpentine flow channels was investigated numerically using computational fluid dynamics (CFD), and experimentally using particle image velocimetry (PIV) techniques. The velocity profile simulated by the CFD model was evaluated by PIV. Rectangular, tapered, and round-bottomed flow channels were compared with respect to mixing and water management capabilities, and pressure drop. The CFD model was further developed to account for chemical reaction on the cathode side to determine which channel configuration is most effective in reactant conversion on the cathode side. The results of this work could be applied to optimizing fuel cell flow channel design.

PAPER 23B.4 — 17:00

EFFECTS OF TRANSPORT LIMITATIONS AND NON-UNIFORM CATALYST DISTRIBUTIONS IN PEM FUEL CELLS: MODELLING AND NUMERICAL ANALYSIS.

D.H. SCHWARZ and N. DJILALI, University of Victoria, Canada

The performance of PEM fuel cells depends on the composition and structure of the catalyst layers. Experimental observations reveal that state-of-the-art catalyst layers consist of microporous agglomerates of carbon-supported catalyst sites bound together by polymer electrolyte. In between the agglomerates are macropores which provide pathways for the transport of gaseous reactants. The active surface is limited to the catalyst sites located on the surfaces of the agglomerates in contact with polymer electrolyte. Improving the performance of PEM fuel cells depends on the

optimisation of catalyst layer composition and structure for large reaction surfaces. This optimization requires a detailed modelling of the reactions and mass-transport in catalyst layers in order to find ways to increase the effectiveness of the catalyst layers for a given precious

metal loading. In this work, three-dimensional, multicomponent and multiphase transport computations are performed using a CFD code (FLUENT™) with a new PEM fuel cell module, which has been further improved by taking into account the detailed composition and structure of the catalyst layers using a multiple thin-film agglomerate model. In this model, it is assumed that thin films of polymer electrolyte and liquid water surround the catalyst sites and therefore that the reactants in the gas phase must dissolve into the water and diffuse across both the water and polymer electrolyte films, before reacting at catalyst sites on the surfaces of the agglomerates in contact with polymer electrolyte. The effects of the resulting transport limitations are investigated, by varying parameters associated with the water and polymer electrolyte films.

From previous modelling studies, it is well known that the distribution of the electrochemical reactions in the catalyst layers is highly dependent on the complex interaction of activation and ohmic effects, as well as contributions from transport limitations and variations in local and overall current density. Available data on catalyst layer composition and structure are used in CFD computations to predict reaction rate distributions in the catalyst layers. Based on these results, variations in local catalyst loading are implemented in CFD computations for a given overall catalyst loading in an attempt to improve PEM fuel cell performance.

PAPER 23B.5 — 17:20

NUMERICAL ANALYSIS OF ELECTRON TRANSPORT AND MASS TRANSFER IN THE GAS DIFFUSION LAYER OF PEMFC

P. C. SUI and N. DJILALI, University of Victoria, Canada

A numerical investigation and parametric study of the coupled electrical conduction and mass diffusion in the gas diffusion electrode (GDL) of a proton exchange membrane fuel cell (PEMFC) are reported in this paper. The coupled transport is solved within a 2-D, “under-the-rib” cross-sectional area of the cathode GDL. The current density on the GDL-catalyst layer interface, which constitutes one of the boundaries of the GDL domain, and which reflects the activation overpotential in the catalyst layer and the ohmic loss in the membrane, is solved iteratively using a novel numerical algorithm. A parametric study is conducted to examine the effects on current density distribution of a variety of fuel cell operating conditions (current density, oxygen concentration) as well as design factors such as GDL geometry, anisotropic transport properties, contact resistance, and deformation under the collector plate landing area. A heuristic model for liquid water transport is also included to assess the effects due to flooding. The numerical analysis shows that depending on the characteristic lengths of electrical conduction vs. mass diffusion in the GDL, the current density distribution under the landing can be dictated by either electron transport or mass transport, and significantly different current distributions are achieved. The present study also provides guidelines to practical design issues such as the dimensions of landing and gas channel as well as selection of GDL materials to minimize current gradients in a GDL.