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Three-dimensional proton exchange membrane fuel cell model: Comparison of double channel and open pore cellular foam flow plates

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ABSTRACT

This study develops a unique three-dimensional computational fluid dynamic electrochemical model for open pore cellular foam material as a flow plate, comparing it to a double channel flow plate and experimental results, researching its application as an alternative to conventional flow plate materials in proton exchange membrane fuel cells.

Using the same membrane electrode assembly and operating parameters, the model simulations, including hydrogen and oxygen distribution and water activity, are examined. IV-curves obtained from the model and experimentally, are analysed and the results are discussed. The model is validated by comparing simulated IV-curve results against experimental results, and model limitations are identified.

The results indicate that the open pore cellular foam material flow plate distributes both hydrogen and oxygen more evenly from inlet to outlet through the fuel cell, when compared to the double channel fuel cell, outperforming it in both simulated and experimental runs.

1. Introduction

The PEM (proton exchange membrane) fuel cell is a low temperature electrochemical device that offers a promising, possibly green, alternative to traditional power sources, and other fuel cell types, in many applications [1–3].

Simulation results from electrochemical PEM fuel cell models can assist in analysing the chemical reactions within the fuel cell and it aims to gain a more detailed understanding, prediction, control and optimisation of the transport effects, liquid formation and electrochemical activities in PEM fuel cells [4]. The first computational models of PEM fuel cells were recorded in the early 1990s, with most models being one dimensional, isothermal and focussing on the electrode, catalyst layer and membrane [5,6]. The late 1990's saw the dawn of more advanced and complex PEM fuel cell modelling, 2-D models were first studied and then 3-D models, with multiphase flow following [7]. Single and two phase flow regimes were classified by current density according to the appearance of water at the MEA (membrane electrode assembly) interface. Extensive research has occurred in the 3-D modelling of PEM fuel cells in recent years. Researchers have modelled many different GDL (gas diffusion layer) materials and thicknesses [8–10] and used various membrane and water models [11,12], in single phase and multiphase flows [13–15], to optimise fuel cell performance. Researchers have also modelled straight, serpentine and tapered flow plates. Within these models, further researchers have performed analysis of PEM fuel cells, modifying the flow field configurations and even channel rib depth, height and aspect ratio [16–18]. With the aid of models and experimentation results it has been identified that one of the key strategies for improving the performance of the PEM fuel cell is the effective design of the flow plate [19]. By improving the design, layout and configuration of the flow plate with the use of low-cost lightweight construction materials and optimal fabrication methods, the weight, volume and cost of a PEM fuel cell stack can be reduced significantly [20].

OPCF (open pore cellular foam) materials are an alternative material to machined graphite materials that have been recently used as flow plates [21–25]. OPCF materials have an open pore structure composed of isotropic pores which are connected to each other by ligaments. The array of pores form a solid homogenous matrix, having the same properties of the parent material but at the

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fraction of the weight. These materials can be manufactured by various processes, casting, foaming, sintering, metal vapour deposition, 3-D printing, etc; according to the size of pore required and state of matter in which the metal is processed [26–28]. A number of researchers [29–31], have developed computational fluid dynamic models and studied fluid flow, pressure drop and thermal characteristics in different environments, however none have developed suitable models and electrochemically modelled a fuel cell with a foam flow plate. Developing models and techniques to model these materials is important to further develop fuel cell technology. Carton & Olabi [32] recently developed a RUCS (representative unit cell structure) model for OPCF material, approximated by a dodecahedron, researching its application as an alternative to conventional PEM fuel cell flow plates. The model gave satisfactory results for pressure drop through the OPCFs, which matched with experimental and mathematical models.

The present study further develops a RUCS, developed by Carton & Olabi, within a 3-D PEM fuel cell electrochemical model. The aim of the study is to compare two PEM fuel cell models; a DCh (double channel) () flow plate PEM fuel cell with an OPCF (open pore cellular foam) flow plate PEM fuel cell, both using the same MEA (membrane electrode assembly) and optimised operating parameters.

Simulations are completed on the DCh and OPCF PEM fuel cells and the results are compared against experimental data (polarisation curves obtained experimentally). Effective flow plate design using OPCF flow plate designs are validated and the results are discussed.

2. Electrochemical model development

Recently, three-dimensional CFD (computational fluid dynamic) models have been developed by taking full advantage of different commercial CFD software packages such as Fluent, Open-Foam, CFX, Star-CD and CFDRC, etc. The PEM fuel cell module is an extra set of equations, to the normal CFD equations, that have been defined by Fluent Inc., for the modelling of PEM Fuel cells. The Fluent PEM fuel cell module is comprised of several UDFs (user defined functions) and a GUI (graphical user interface). The electrochemical reactions occurring on the catalyst are modelled through various source terms while other model parameters are handled through the user interface.

Schematic diagrams of the PEM fuel cell models used in this analysis are illustrated in Figs. 1 and 2. Each model consists of cathode and anode gas flow regions, catalyst layers, gas diffusion layers and current collectors (flow plates). In the PEM fuel cell module two electric potential fields are solved. One potential is solved in the membrane and catalyst layers. The other is solved in the catalyst layers, the diffusion layers and the current collectors. Surface reactions on the porous catalyst region are solved and the reaction diffusion balance is applied to compute the rates. Based on the cell voltage that the user defines, the current density value is computed. Alternatively, a cell voltage can be computed based on a user defined average current density. The liquid water saturation, s, and the water content, λ, are also solved as user-defined scalars [33] (Refer to the Appendix for more detail on the equations defined by Fluent Inc. PEM fuel cell module). The assumptions made in developing the model are as follows:

- Ideal gas mixtures
- Incompressible and Laminar flow
- Isotropic and homogeneous porous electrodes, catalyst layers and membrane
- Isothermal operation
- Negligible ohmic resistance at porous electrodes and current collectors

The model was imported in to commercial software, Ansys mesh, boundary conditions were added, and it was meshed using either quadrilateral mesh elements or hybrid elements by specifying the minimum edge length. The CFD software version used in this study can only be used with cases containing less than 512,000 elements and so each model has restrictions on its physical dimensions and mesh size. Final models contained between 300,000 and 400,000 elements, course enough not to exceed the limit or computational power or time available, but fine enough to give acceptable results, clarified by grid independence analysis. In this study a grid 20% finer than the base grid was used for a comparison analysis of each mesh. Polarisation curves showed no significant difference in performance of the models; therefore the base mesh was used as it reduced the number of nodes saving computational time.

In order for the CFD analysis software to recognise the PEM fuel cell model, the zone types must be clearly modelled using Ansys Mesh. Two zone types that need to be specified are boundary and continuum zone types. Boundary-type specifications define the physical and operational characteristics of the fuel cell at those topological entities that represent model boundaries. Continuum zone types define the physical characteristics of the model within specified regions of its domain. For the PEM fuel cell module only the cathode and anode collector are specified as the solid continuum-types, this also simplifies the model [33]. The boundary types are specified as faces while the continuum zone types are the volumes of each component. The boundary zones specified for both the DCh and OPCF electrochemical models are detailed in Table 1.

With all the zones specified, the mesh was exported ready for analysing. The PEM fuel cell model parameters are set and properties assigned to the relevant regions of the fuel cell before defining the boundary conditions. In order to run the model a minimum number of parameters have to be available to the user; obtained from the fuel cell specifications, experimentation, electrochemistry calculations and existing material properties. A full list of the input parameters for both models is detailed in Tables 2 and 3. The analysis was carried out at loading conditions of 0.85 V (low current density), 0.75 V, 0.65 V and 0.55 V (high current density) and polarisation curves (I–V curve) with a power density curve are plotted. Several key phenomena were monitored during each simulation, until convergence, including continuity and velocity, and checks were made to ensure steady state and low residual RMS error. Flux reports were also analysed; the sum of the flux at the inlet should closely match the flux at the outlet.

2.1. Double channel electrochemical model development

To reduce complexity and computational demand, a section of the complete double channel flow plate is used for the selected computational domain, see Fig. 1.

The domain consists of two, straight, counter flow, channels, each 1 mm × 1 mm × 37 mm. The dimensions of the full domain are 5.5 mm × 5 mm × 37 mm in the x, y and z directions, respectively. The cross sectional area of the membrane electrode assembly is consequently 192.5 mm^2, the area used in obtaining the current density.

The most suitable 3-D mesh for the double channel model is the quad sub-map mesh, which specifies that the mesh includes only quadrilateral mesh elements. This mesh structure is particularly suited for this type of solution because it increases the rate of convergence, increases solution accuracy and reduces the CPU time required.

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