# 3-D Modelling of a Proton Exchange Membrane Fuel Cell with Anisotropic Material Properties

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## Abstract

Fuel cell performance is dependent on a strongly coupled interaction taking place between convection, diffusion, electrochemical reactions, membrane water transport and heat transfer. Furthermore, the thermal and electrical properties of materials used in fuel cells are anisotropic. In addition, during normal operation of the fuel cell, the two phases of water are present both in the porous gas diffusion layers and in the channels of the oxidant and the fuel. To properly model the effect of all these phenomena in three dimensions with all the couplings and the anisotropy of the material properties presents a significant challenge. In this paper, aspects of a CFD-based modelling approach will be presented. Such an approach takes into account the coupling of the above phenomena by making some engineering assumptions in handling of the individual phenomenon. It is also able to treat the material anisotropy and different material properties used in the fuel cell and thus can be used as an engineering tool for understanding the impact of material changes in future designs. Typical results from these coupled 3-D simulations, which account for the anisotropic material properties, are presented. It is concluded that anisotropic properties play an important role in the coupled transport in a PEMFC and thus accurate measurement of these material properties for input in computational models is needed.

## Introduction

Fuel cells are being pursued aggressively as a promising source of clean and renewable power as peaking of oil reserves looms in not so distant future. Several companies and organizations are developing fuel cell solutions for a range of applications of which stationary power generation and automotive applications are major components. Each application tends to have its own unique requirement for fuel cell design and operation. As the cost of development is a common thread in all of these, cutting design cycle times and getting the design right the first time continues to be a major emphasis for all developers. This has increasingly led to aggressive use of modeling, analysis and simulation tools within the industry. These tools at various levels of complexity are being used to study and improve concepts to 3-D designs and further aid in the analysis and troubleshooting of failure mechanisms as brought out by testing. Given that several multi-physical and multi-scale phenomena taking place in a fuel cell are still not fully understood, engineers have built heuristic models for these where needed while universities and other organizations continue to improve on the models to better account for the physics. The objective of this paper is to report on the 3-D modelling of a PEMFC using a simulation tool with anisotropic transport properties for the fuel cell components.

# CFD-based Simulation Tools

Fuel cell modeling approach based on computational fluid dynamics (CFD) offers the engineer the advantage of studying and improving 3-D designs during the design cycle thus ensuring that enough effort is expended to minimize surprises down the line. Typically such CFD-based model solves for the governing conservation equations for mass, momentum, species and energy, which besides being a common backbone to many of the engineering problems, is also a relatively mature subject. Built on this CFD backbone are the additional models for electrochemical reactions, membrane water transport, electronic and ionic potential, and a saturation model to account for the two phase flow in PEMFC. These models are continuously being improved and are being calibrated using test data. The methodology of employing CFD for PEMFC modelling can be found in [2], among many others. The major advantage of using a comprehensive, 3-D CFD tool for PEMFC modelling over reduced dimension or simplified models is the high fidelity of the computational results. Although the computational time for CFD is often demanding, large scale parallel simulations using computer clusters have been demonstrated. In addition to being a tool for analysis, CFD-based tools can be modified to become a design tool, cf. [7].

# Anisotropic Properties of Materials Used in a PEMFC

Most of the components of a PEMFC have anisotropic transport properties. The gas diffusion layer (GDL) in particular shows significant differences in the transport of electricity and heat in the in-plane and the through-plane directions. The catalyst layer is a composite material that is constructed by two networks (electrolyte and carbon black respectively), which shows some degree of anisotropy due to fabrication processes and also possibly due to preferred material orientation. The bipolar plate that is made of graphite powder and resin binder has some flaky structure that makes its transport properties anisotropic. Among all these materials, the anisotropy in the GDL is believed to be the most influential because of its fibrous structure as well as the fact that it is subject to discontinuous property change on one boundary, i.e. on the side that is in contact with the bipolar plate, cf. [3]. Furthermore, part of the GDL on the GDL-bipolar plate interface is under compression and the transport through such region is complicated, cf. [1] and [8]. Owing to the complexity of coupled transport phenomena, analysis on the effects due to anisotropy in transport properties of the materials in a PEMFC is best assisted by employing a simulation tool.

# Results and Discussion

The transport property for a thermal or electrical conduction equation takes the form of a tensor:

$$\bar{k} \equiv \begin{vmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{vmatrix} \tag{1}$$

For a conventional plate-and-frame type of membrane electrode assembly (MEA) with coordinates X and Z as the in-plane direction and Y as the through-plane direction, we assume the

transport is limited in both planes, i.e. only diagonal terms in the matrix remain. For a PEMFC problem, the anisotropy should appear in the conservation of species (diffusivity), momentum (permeability), energy (heat conductivity) and potential (electrical conductivity).
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The baseline case used for the present study is a CFD model based on Ballard hardware. A commercial CFD software, CFD-ACE+, is used in the present study. The software with its capabilities for fuel cell simulations solves a complete set of conservation equations, which includes solution of conservation of charged species, water transport across the membrane, as well as transport of liquid water in porous media. The properties and model parameters used are obtained from validation with experimental data from [5]. The electrical conductivity used in the baseline case is isotropic and set to be 200 $(\Omega m)^{-1}$. A sensitivity analysis of numerical predictions for a Ballard hardware due to these properties shows that predicted performance is more sensitive to electrical conductivity than to thermal conductivity. Figure 2 shows the cell voltage predictions as a function of the anisotropy ratio, i.e. the ratio of the in-plane value versus the through-plane value. The through-plane value is kept constant for these calculations. One can see as the in-plane electrical conductivity is increased, the cell voltage increases because the ohmic loss in the GDL is reduced. For the thermal conductivity, the in-plane values have negligible impact on the overall cell voltage until it is reduced significantly, at which conditions the cell temperature rises because the transfer of the heat generated in the MEA is limited by the through-plane conduction and results into a higher temperature of the cell. The cell voltage appears to increase with increased cell temperature primarily due to a high electrical conductivity of the membrane at higher temperature.

Figure 3 shows a cross section plot of electrical potential and current flow in the cathode side and the MEA. The current from the catalyst layer sees a narrower flow path as it approaches the land area where the bipolar plate is in contact with the GDL. The in-plane resistance for current is relatively higher than the through-plane resistance, therefore a high current is seen near the area underneath the land. When the in-plane conductivity is set to two orders of magnitude higher than the baseline value while keeping the same through-plane conductivity as in the baseline, the current distribution changes significantly, cf. bottom of Fig. 3. In this case because the in-plane conduction is no longer important, the conduction becomes like one-dimensional dominated by the through-plane conduction. Figure 4 shows the through-plane current profile on the GDL/catalyst layer interface for different degree of anisotropy of electrical conductivity. The current profile for the isotropic case appears to be distorted towards the land area. As the in-plane conductivity is increased, the current profile becomes less distorted. As the disparity between the in-plane and through-plane conductivity increases, the transport in the in-plane becomes less dominating. As a result, the distribution of current density in the GDL is more uniform. In fact, when the gradient of electrical potential in the lateral direction diminishes, the distribution of current density on the GDL/catalyst layer interface will be likely dictated by mass transport in the GDL, cf. [6].

Figure 5 shows the temperature field of the MEA for isotropic (top) and anisotropic thermal conductivities. For the isotropic case the thermal conductivity is 2 W/m-k. For the anisotropic case, the in-plane conductivity is set to 100 W/m-k while the through-plane value is kept as 2 W/m-k. One can see that for the anisotropic case the temperature gradient as well as the MEA temperature are both lower than the isotropic case. Figure 6 shows a comparison of predicted polarization curves using isotropic and anisotropic electrical conductivity. The anisotropic case has the same through-plane

conductivity as the isotropic case while its in-plane conductivity is one order of magnitude higher than the isotropic case. The reduced ohmic loss in the in-plane direction of the GDL results in a slightly higher cell voltage.

## Conclusions

In the present study we report on comprehensive, 3-D modelling using a CFD tool for PEMFC, which includes specification of anisotropic transport properties for the MEA. It is demonstrated in the numerical predictions that the cell performance is sensitive to the anisotropic electrical conductivity. For the cases tested for Ballard hardware, it is shown that when the in-plane electrical conductivity is increased, the through-plane current density predictions on the GDL/catalyst layer becomes less distorted by the presence of the land area and the cell voltage increases because of reduced ohmic loss. It is also shown that the numerical prediction for cell voltage is not sensitive to the anisotropic thermal conductivity until the in-plane conductivity is substantially reduced. The present study indicates the importance of anisotropic transport properties and calls for measurement data for the materials used in the PEMFC.
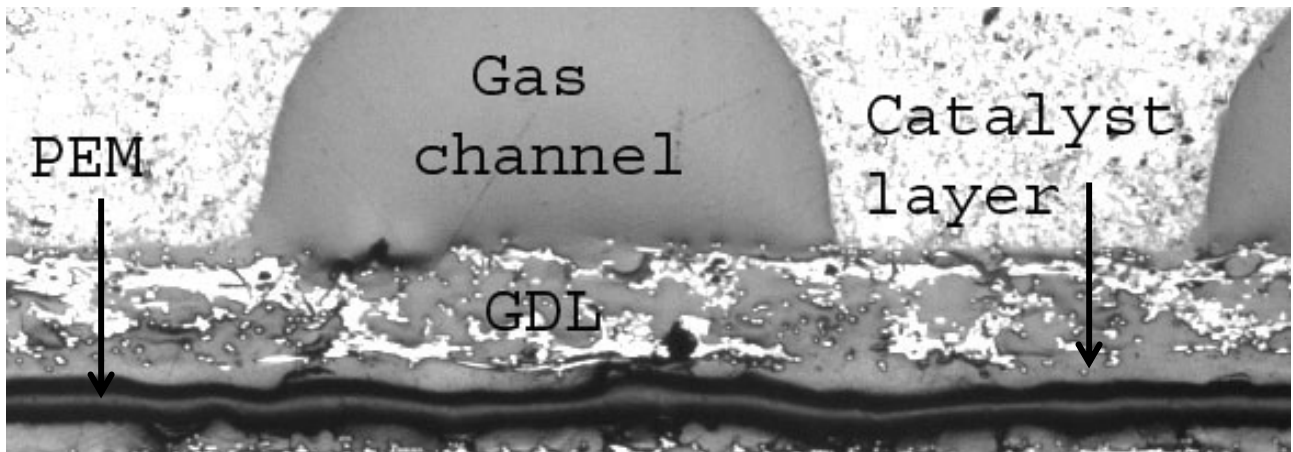
## Acknowledgement
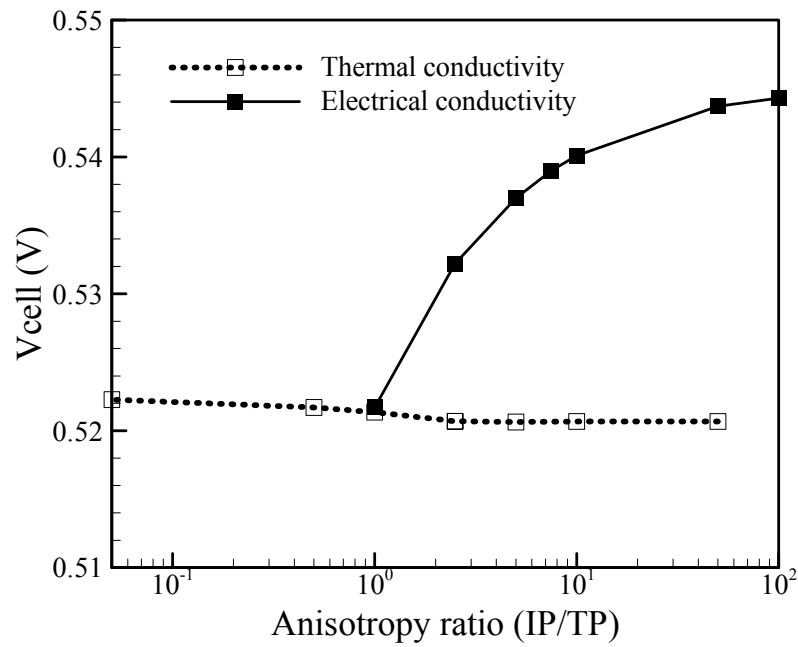
Figure 1. Cross sectional cut of an MEA

Figure 2. Sensitivity of predicted cell voltage due to anisotropy of electrical and thermal conductivities
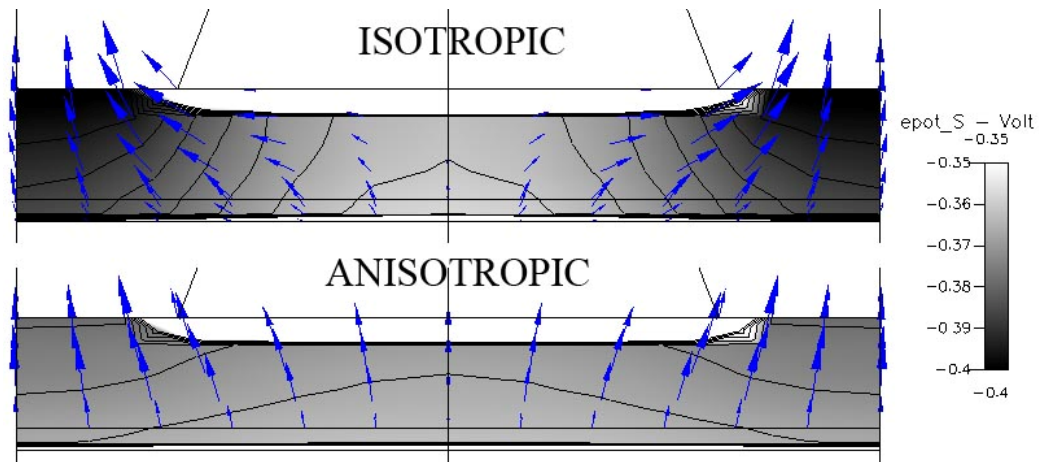(IP= in-plane, TP= through-plane)



Figure 3. Electrical potential distribution and current vectors in the cathodic catalyst layer and GDL
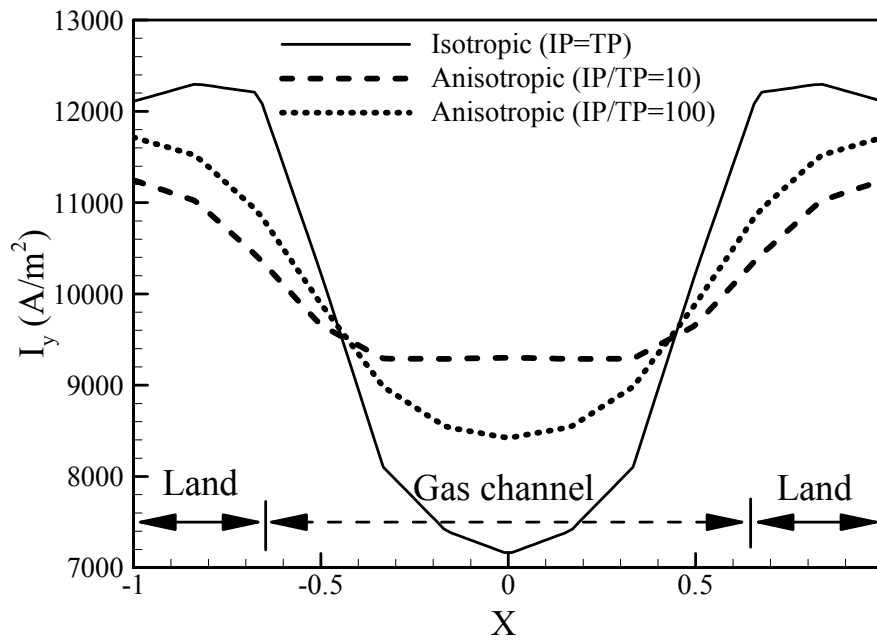
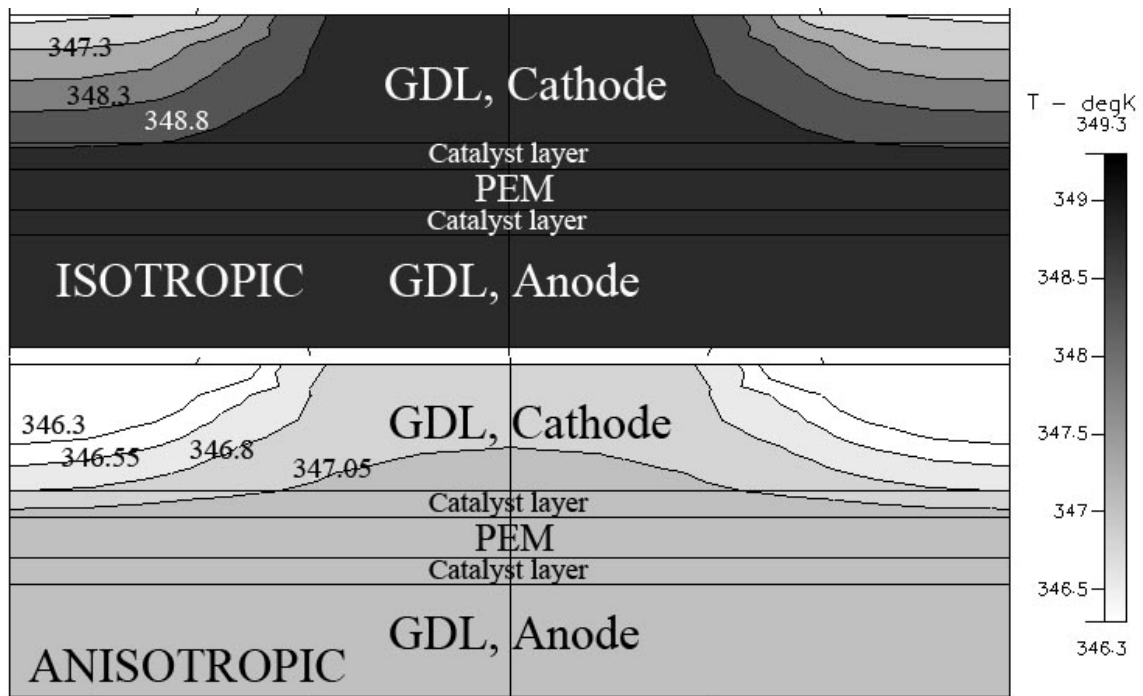Figure 4. Predicted profiles of through-plane current on cathode GDL/catalyst layer interface
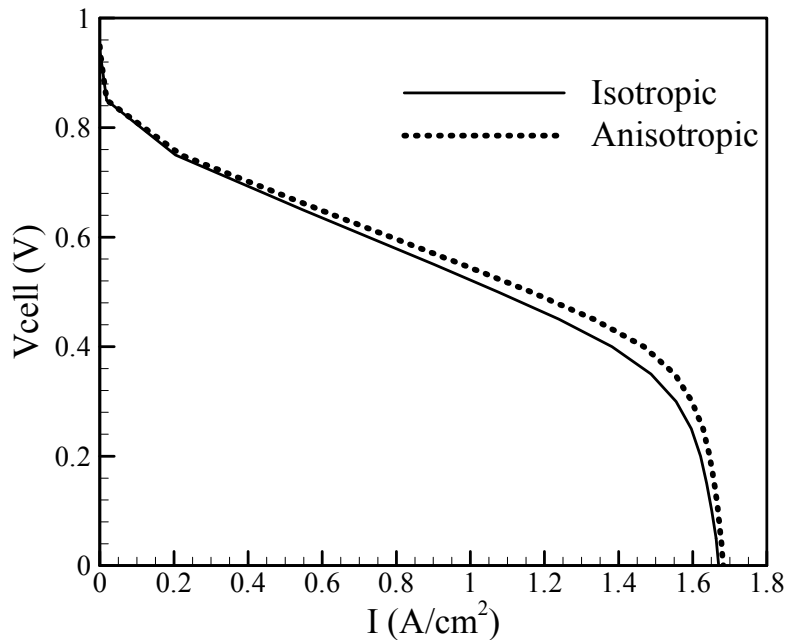


Figure 5. Predicted temperature of the MEA

Figure 6. Polarization curve predictions

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