Macro-Scale Analysis of Large Scale PEM Fuel Cell Flow-Fields for Automotive Applications

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The objective of this work is to establish the design principles for a proton exchange membrane fuel cell in automotive applications. In this work, the macro-scale analysis was considered to create the overall design principle. A combination of experiments and numerical simulations were carried out and the results analyzed to enhance understanding of the behavior of the large-scale 300-cm² proton exchange membrane fuel cell under automotive operations. A three-dimensional computational fluid dynamics-based methodology was used to predict such as the current and temperature distributions of this design as a function of anode relative humidity. The effect of flow direction and the cooling pattern on this design was also taken into account to enhance the understanding for this selected flow-field design. The predictions show that the gas flow and cooling directions are important dependent variables that can impact the overall performance and local distributions.

As the increased number of power generators utilizing fossil fuel energy increases in many applications, the necessity for alternatives to the internal-combustion engine become even more obvious. Automakers and industrial developers are investigating many ways to significantly reduce emissions for stationary and transportation applications. Proton Exchange Membrane Fuel Cells (PEMFCs) are now widely seen as a possibility. Distributions in reactant species concentration in a PEMFC cause distributions in local current density, temperature and water over the area of a PEMFC. These can lead to locally negative effects such as excessive hydration or dehydration in the PEMFC thus causing stresses in effective regions of the fuel cell. Changing operating conditions and design parameters including their properties inside PEMFC system such as flow field configurations, gas diffusion layer (GDL), and membrane electrode assembly (MEA) could vary uniformity in distribution and impact the fuel cell performance and durability.1–16

The inherent non-linearity of the equations governing PEMFC performance on a three-dimensional level requires iterative solution techniques. Solving a full three-dimensional CFD model for the flow channel and diffusion layers of a PEMFC shows important interactions of porous media and flow-field design that affect distributions of current, temperature, and species transport as discussed in numerous literature for the past ten years.1–22 This type of model lends itself well to investigating the physics inside full-scale PEMFCs.1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17

In this work, three-dimensional (3D) CFD simulations of PEMFC were performed for a full size single cell with 300 cm² active area. An ultimate purpose of this study was to establish a model-based engineering capability to design the PEMFC for targeted applications. For this time, robustness of the fuel cell performance was investigated with various operating conditions which can impact the water management problems in the PEMFC.23–26 Especially, relative humidity in anode and cathode operating conditions are sensitive to water management problems. This CFD based two-phase fuel cell performance model was considered to be suitable to cover these problems. The effect of flow direction of reactant gases and the cooling flow patterns were also taken into account to this macro-scale fuel cell performance model.

Model Development

Figure 1 shows model geometry of the fuel cell flow-field and its components used in this study. It has 62 channels in both the anode and cathode in parallel fashion on a 300-cm² active area. It is noted that the straight-parallel flow-field is commonly used nowadays for large scale PEMFC. This flow-field is designed to avoid hot spots at the bending areas of serpentine under high current density and to eliminate water trapped at the same location under low current density. The geometry of the fuel cell arrangement modeled in this work consists of two flow channels separated by diffusion layers and MEA. The flow path is approximately 25.3 centimeters long in the axial direction for both sides. The channel dimension of both the anode and cathode are shown in Table I. Figure 2 presents the computational meshes created in this work for numerical simulation. The mesh was designed with hybrid patterns where the plate and channel were unstructured meshes and GDL and MEA were structured meshes. A total of 12 million cells (elements) were used to model the fuel cell.

A computational continuum mechanics (CCM) technique based on a commercial flow solver, STAR-CD 4.18, was used to solve the coupled governing equations.27 These equations include mass, momentum, energy, and species transport equations. This software has an add-on module called expert system of proton exchange membrane fuel cell (ES-PEMFC) version 2.51 that incorporates multi-physics of PEMFC.28,29 These require the source terms for species transport, multiphase flow, and heat generation equations.1–12 Also, ES-PEMFC accounted for the flux of protons and water across the membrane.30 The material properties, and operational parameters used for this model are shown in Table II. The operating condition of stack experiments and model simulation are shown in Table III. They are used as the boundary conditions and initial conditions for the model. The cell temperature and the system pressure given in Table III are the inlet values or they can be called as the operating temperature and the operating system pressure, respectively. The relative humidity of gas increases when the current density is increased. This increase of current density generates a higher gas flow rate in order to maintain utilization of gas and therefore the relative humidity of gas can be
Table I. Channel geometries.

| Criteria                  | Anode Channel | Cathode Channel |
|---------------------------|---------------|-----------------|
| Depth (mm)                | 0.40          | 0.40            |
| Draft Angle (deg)         | 45            | 35              |
| Top Bend Radius (mm)      | 0.46          | 0.30            |
| Bottom Bend Radius (mm)   | 0.20          | 0.20            |
| Bottom Flat (mm)          | 0.300         | 0.549           |
| Top Landing (mm)          | 0.303         | 0.320           |
| Plate Thickness (mm)      | 0.1           | 0.1             |
| # of Channels             | 62            | 62              |
| Span                      | 1.647         | 1.630           |
| VS-Span                   | 1.633         | 1.482           |

risen. Table III also gives the detail gas concentration and temperature boundary at the wall as it represented the cooling temperature at each current density. This model has been validated with experimental data and the results were satisfied in polarization data, water balance data, and local current mapping data.\textsuperscript{1,11,12,29}

The solution procedure used in this solver is based on a SIMPLE algorithm\textsuperscript{30} with algebraic multigrid (AMG) method.\textsuperscript{31,32} At each iteration, three momentum equations corresponding to three coordinate grids are solved, followed by a pressure correction equation that performs a mass balance. Enthalpy and species transport equations are solved after the bulk flow calculation. The mixture properties at each control volume are calculated based on the local species content. Therefore, the density and viscosity of the mixtures in the anode and cathode flow channels vary from control volume to another.

In order to perform the calculations, STAR-HPC, a parallel solver, was used. STAR-HPC uses a domain decomposition approach to divide the computational geometry among the computational nodes as shown in Figure 3. The jobs were run on 6 processors running Linux. The computational domains pass information to and from the other domains using MPICH, an open source implementation of the MPICH message passing libraries, during iterations, thus the entire domain is
directions with opposite cooling directions. Finally, the change of inlet same direction of cathode inlet. Figures 4b and 4c are the counter flow co-flow of anode and cathode. The cooling pattern was started with the cooling directions. The baseline direction as shown in Figure 4a was then discussed. Figure 4 shows the direction of gas flow with different of the cooling pattern on the performance and local distributions was reported and discussed. The effects of flow direction and the direction run in as little as 600 iterations.

Solving the current convergence is determined by a 1% closure of the global mass and species balances. For this study, all cases were run with constant stoichiometry at a given current given in Table III. Fixing the current and stoichiometry at given humidification and outlet pressure conditions for a PEMFC yields inlet flow rates and mole fractions for both the anode and cathode. A shoot and correct method is then used to converge on the cell voltage. When a value for the cell voltage is supposed, the model iterates to find the species and electrochemistry distributions. The current from the cell can then be calculated from these distributions and if the current from the cell does not match the current for which the inlet flow rates were set, then the cell voltage is adjusted. The amount of iterations to meet the convergence criteria varies between models and conditions; however, it generally occurs around 600–700 iterations. At the start of each current condition the model was run for 300 iterations as a non-reacting flow problem to get better convergence for the mass balance. Generally, it takes around 2000 iterations to run 1 current condition for a model; however, if the cell voltage is well-known, the model could be run in as little as 600 iterations.

In this work, model validation against the experimental data was reported and discussed. The effects of flow direction and the direction of the cooling pattern on the performance and local distributions was then discussed. Figure 4 shows the direction of gas flow with different cooling directions. The baseline direction as shown in Figure 4a was co-flow of anode and cathode. The cooling pattern was started with the same direction of cathode inlet. Figures 4b and 4c are the counter flow directions with opposite cooling directions. Finally, the change of inlet

### Table II. Assumption of operating parameters and material properties in the model.

| Current Collector | Value |
|-------------------|-------|
| Stainless Steel: Thermal conductivity (W/m-K) | 16.3 |
| GDL | |
| Thickness after compression (μm) | 190 |
| Permeability (m²) | 2.0e-11 |
| Porosity after compression (%) | 74 |
| MacMullin Number | 3.9 |
| Thermal conductivity (W/m-K) | 0.25 |
| Membrane Electrode Assembly | |
| Thickness (μm) (including 12.5 μm thickness of catalyst layer) | 30 |
| Thermal conductivity (W/m-K) | 0.15 |
| Dry membrane density (g/cm³) | 2.0 |
| Equivalent weight of dry membrane (g/mol) | 1100 |
| Cathode exchange current density (A/cm²) | 0.05 |
| Cathode transfer coefficient | 0.7 |
| Anode exchange current density (A/cm²) | 0.5 |
| Anode transfer coefficient | 1.4 |

### Table III. Operating condition.

| Current Density (A/cm²) | 0 | 0.01 | 0.03 | 0.05 | 0.1 | 0.3 | 0.6 | 0.8 | 1.0 | 1.2 | 1.4 |
|-------------------------|---|------|------|------|-----|-----|-----|-----|-----|-----|-----|
| Fuel | | | | | | | | | | | |
| H₂ Concentration | % | 63% | 63% | 69% | 74% | 77% | 80% | 82% | 83% | 84% | 86% |
| H₂ Stoic | - | 7.4 | 7.4 | 3 | 2.1 | 1.8 | 1.9 | 1.7 | 1.7 | 1.7 | 1.7 |
| Fuel pressure inlet | atm | 1.2 | 1.23 | 1.23 | 1.23 | 1.2 | 1.2 | 1.6 | 2 | 2.3 | 2.6 |
| Dew Point inlet | ºC | 53 | 53 | 53 | 54.8 | 55 | 56 | 57 | 58 | 58 | 59 |
| Fuel Inlet RH | % | 72% | 72% | 72% | 78% | 79% | 82% | 88% | 90% | 92% | 93% |
| Air | | | | | | | | | | | |
| Air Stoic | - | 10 | 10 | 3.1 | 1.9 | 1.8 | 1.8 | 1.8 | 1.8 | 1.7 | 1.7 |
| Air pressure inlet | atm | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 | 1.4 | 1.4 | 2 | 2.3 | 2.5 |
| Dew Point inlet | ºC | 55 | 55.3 | 55.3 | 55.3 | 55 | 58 | 58 | 58 | 59 | 59 |
| Air Inlet RH | % | 80% | 80% | 80% | 80% | 80% | 92% | 92% | 92% | 92% | 95% |
| Coolant | | | | | | | | | | | |
| Temp inlet | ºC | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 |
| Inlet-Outlet deltaT | ºC | 0 | 0.3 | 1.1 | 2 | 3.5 | 6.6 | 9 | 10 | 11 | 12 |

### Results and Discussion

**Model Validation.**—Figure 5 shows a polarization curve of the single cell and model prediction. The polarization curve was taken with a 20 cells stack and the cell potential is the average of 20 cells. Numerical calculation at 9 points were chosen to cover the entire range of current density (i.e., 0.01, 0.05, 0.1, 0.3, 0.6, 0.8, 1.0, 1.2 and 1.4 A/cm²). With the kinetic parameters provided in Table II, the predictions agree well with experimental results. It is noted, for this experimental setup, the co-current flow direction in both gases and cooling were chosen as shown in Figure 4a. The prediction of local distributions of current density, membrane water content, liquid water, and overpotential at average current density of 1.0 A/cm² are shown in Figure 6. The distribution of local current density on the MEA surface is the highest at the inlet. Then it decreases toward the outlet due to the consumption of the reacting gases. The increase in cathode overpotential from the inlet toward the outlet indicates the transport limitation of oxygen. The membrane water content also increases from the inlet toward the outlet because the water produced from the electrochemical reaction accumulates along the cathode channel and some of the water transports across the membrane from the cathode. Figure 7 presents the gas-liquid concentrations along the channel on both the anode and cathode flow channels. In this case, both hydrogen and oxygen are consumed along the channel due to electrochemical reaction thus the mass fraction of those gases are decreased toward the outlet. There is some liquid water presented in the flow channel of the cathode side but the quantity is not significant. It is noted
that there is uneven water saturation at each cathode channel and the higher saturation are shown at the around center channels and the far right channels. This could be due to the specific manifold design of this flow-field causing the irregular distribution of partial pressure of water at each channel, thus impacting the condensation/evaporation of water.

**The effect of flow direction and cooling pattern on PEMFC performance.**—The flow direction is one of the design valuables used in the fuel cell stack for automobiles. Therefore, the effect of flow direction on the performance in this particular flow-field design are considered. The baseline inlet relative humidity (RH) is chosen for this task. The purpose of this study is to investigate how the overall performance and local distributions are changed when the gases’ flow direction is in the opposite direction from the original (i.e., counter-current flow). Moreover, effect of cooling flow direction is also taken into account. Figures 4b and 4c show the direction of reacting gases in both cathode and anode and the direction of cooling pattern. Therefore there are two cases preformed in this section and the predictions are compared with the original baseline data. The flow direction in Figure 4b is the counter-current flow direction with the cooling flows from cathode to inlet-Outlet deltaT

| Current Density A/cm² | 0  | 0.01 | 0.03 | 0.05 | 0.1 | 0.3 | 0.6 | 0.8 | 1 | 1.2 | 1.4 |
|-----------------------|----|------|------|------|-----|-----|-----|-----|---|-----|----|
| Fuel Inlet RH         | High | 72%  | 72%  | 72%  | 78% | 79% | 82% | 88% | 90%| 92% | 93% |
|                       | Med  | 30%  | 30%  | 30%  | 31% | 31% | 34% | 39% | 41%| 44% | 47% |
|                       | Dry  | 20%  | 20%  | 20%  | 21% | 21% | 24% | 29% | 31%| 34% | 37% |
| Air inlet RH          | Dry  | 20%  | 20%  | 20%  | 20% | 21% | 22% | 24% | 26%| 27% | 29% |
|                       | Coolant Temperature | 6 | 0.3 | 1.1 | 2 | 3.5 | 6.6 | 9 | 10 | 11 | 12 |

**Table IV. Inlet humidity conditions.**

![Figure 4](image_url)  
**Figure 4.** Direction of gas flow for both anode and cathode with different cooling directions.

![Figure 5](image_url)  
**Figure 5.** Validation of polarization curve.
Figure 6. Local distributions on MEA surface at $I_{avg} = 1.0 \text{ A/cm}^2$.

Figure 7. Gas and liquid distributions in the flow channels at $I_{avg} = 1.0 \text{ A/cm}^2$. 
ode inlet location. In this case the temperature is low at the cathode inlet and higher at the anode inlet. Figure 4c also shows the counter-current flow with the cooling flows from the anode inlet, thus giving the lowest temperature at the anode inlet location.

Figure 8 shows the potential comparison at different current densities between those two cases and the baseline of co-current flow direction. From this graph, the overall performance looks similar at the low current densities (i.e., OCV to 0.6 A/cm²). At high current densities starting from 0.6 A/cm², the potential of cooling flow from cathode inlet is the highest following by counter-current flow with the cooling flow from the anode inlet and co-current flow. These predictions indicate that the counter-current flow direction gives the highest performance when compared with the co-current flow under the high inlet RH condition. Further, the comparison of local distributions between those three flow configurations are shown in Figure 9. These local distributions include current density, membrane water content, and cathode liquid water at averaged current density of 1.0 A/cm². From the local current density distribution, all cases show different pattern and also cell potential. It appears that the counter-current flow with the cooling flow in the same direction as the anode inlet gives the most uniform distribution with the highest local value located at the around the middle of the MEA surface. For other two cases, the local distribution shows the maximum value is where the cathode inlet and/or cooling inlet are located and then it decreases toward those outlets.

The distributions of membrane conductivity are also shown in Figure 9. They are similar to the distributions of current density as the co-current flow and the counter-current flow with cooling direction follows anode flow have similar uniformity. But the counter-current flow with cooling’s flow pattern is in the same direction as the cathode flow gives the most non-uniformity with the highest averaged proton conductivity. These predictions of membrane conductivity distribution...
dependence on not only the RH but also the flow direction of the reacting gases and cooling. The cathode liquid water distributions also given in this figure have similar content and they all show the condensation occurs around the half way point of cathode flow toward the exit. The counter-current flow with the cooling flows the same direction of anode inlet has the highest content compared to other cases. The co-current flow shows the least of water condensation in the particular operating condition.

**The effect of inlet RH on PEMFC performance.—** In this section, the sensitivity of anode humidity on the performance and distributions of this flow-filed are studied. The counter-current flow direction with cooling inlet as same direction as cathode inlet are chosen in this work as it represents the typical setup of the fuel cell stack used in automotive applications. This setup also includes the low humidity of air in the cathode side to minimize water flooding in the system. The operating conditions for this study are given in Table IV.

Figures 10a to 10d present the overall predictions of performance, relative humidity at anode outlet, water mass flow rate at the anode outlet, and water flux from anode to cathode per water generation. For Figure 10a of overall performance, Dry/Dry condition shows the worst performance. It is noted that Dry RH in this work means the relative humidity of inlet gas is lower than 50%. High RH/Dry and medium (Med) RH/Dry gives similar performance and they are significantly higher than Dry/Dry conditions especially when the current density is greater than 0.6 A/cm². With these specific setups, Med RH condition may be suitable for counter-current flow. The RH change and the water flow rate plots at the anode outlet are presented in Figures 10b and 10c, respectively. The RH of the gas at the anode outlet is increasing when the current is increased until the current density is greater than 1.2 A/cm² then the anode outlet’s RH decreases especially for the Dry/Dry case. This could be due the water transport across the membrane and the significant increase of temperature in the gas channel at the outlet. Dry/Dry shows the least water coming out of the anode flow. Figure 10d shows the ratio between the water flux across membrane from anode to cathode and the water generation. The prediction reveals that the Dry/Dry shows more uncertainty of water transport across the membrane compared to other operating conditions.

Figure 11 presents the current density distributions with different anode humidity mentioned above at two different averaged current density of 1.0 A/cm² and 2.0 A/cm². Current distributions look similar for High/Dry, Med/Dry, and Dry/Dry RH for lower current density.
Conclusions

It can be concluded that by changing the gas flow pattern it can affect the performance and uniformity. With this design, the counter-current flow direction gives better performance than the co-current flow direction in particular at the well humidified condition. This prediction agrees well with the experimental results done at Ford Motor Company. It is also concluded that the cooling flow direction and where the low temperature of cooling enter the system is also one of the dependent variables that impact the fuel cell performance and the distributions. Under counter-current flow and well humidified gas stream, the cooling flows in the same direction of the cathode inlet gives the best performance but less uniform distributions when compared with the cooling flows in the same direction as the anode inlet. However, if the operating condition changes such as humidity and/or stoichiometry, the results will be changed with different conclusion. The change in anode humidity shows less sensitive to the performance and distributions at High RH and Med RH. The Dry RH shows more sensitive when the current density is high. Dry/Dry shows more uncertainty for water transport across the membrane compared to other operating conditions.

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Figure 11. The effect of anode humidity with dry cathode on current density distribution (A/cm²) at average current density of a) 1.0 A/cm² and b) 2.0 A/cm².

(i.e., 1.0 A/cm²). For higher current density (i.e., 2.0 A/cm²), the Dry/Dry condition gives much lower performance and the highest non-uniform distribution compared to High/Dry and Med/Dry RH.