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# Simulation of an innovative polymer electrolyte membrane fuel cell design for self-control thermal management

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ABSTRACT

Two novel fuel cell designs attempt to improve efficiency and reduce the balance of plant weight by implementing a square hole through the center of the bipolar plates. Air is forced through the square hole for the purpose of oxygen delivery, water removal, and stack cooling. This study demonstrates, for the two novel designs, a more even temperature distribution and hot spots away from the center of the bipolar plates. This reduces the number and size of components required to effectively run the system, thus reducing the weight of the balance of plant. Four simulations are presented in this paper, with inlet gases and initial cell temperature set to 333 K. The maximum temperature for case 1 without cooling is 347.97 K, case 1 with water cooling is 335.29 K, case 2 with forced air cooling is 339.42 K, and case 3 with forced air cooling is 335.13 K.



## 1. Introduction

Fuel cells are very complex systems that require special materials and manufacturing techniques. This makes it expensive to build and test different fuel cell designs. Using computational fluid dynamics (CFD) software, it is possible to alleviate some of the time and expense involved in testing fuel cell designs. By building virtual models of desired designs and simulating them, a selection can be made before anything is purchased. In addition, simulations are a good platform from which to evaluate experimental data. Reasons for good or poor performance can be more readily identified. When optimizing a fuel cell, operating conditions must be balanced. For instance, increasing the air flow rate will always provide more oxygen and/or hydrogen for reaction; however, too much air flow can destroy the thin inner layers and bring about challenges in keeping the fuel cell sealed. Optimization is of key importance to the advancement of fuel cells, as it increases performance and efficiency, making fuel cells more viable economically.

To advance fuel cell technology, it is critical to effectively simulate fuel cell fluid transport and electrochemical reactions according to Wang et al. [1]. The main expense in a fuel cell currently is the platinum loading of the activation layer on

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**Nomenclature**

| | |
|---|---|
| $A_c$ | cathodic tafel slope, V |
| $cH_2\_ref$ | hydrogen reference concentration, mol $m^{-3}$ |
| $chcs.c\_wH_2$ | hydrogen molar concentration, mol $m^{-3}$ |
| $chcs2.c\_wO_2$ | oxygen molar concentration, mol $m^{-3}$ |
| $cO_2\_ref$ | oxygen reference concentration, mol $m^{-3}$ |
| $C_p$ | heat capacity at constant pressure, J $kg^{-1}$ $K^{-1}$ |
| $F$ | Faraday's constant; 96,487, C $mol^{-1}$ |
| $i_l$ | electrolyte current density, A $m^{-2}$ |
| $i_{loc}$ | local charge transfer current density, A $m^{-2}$ |
| $i_0$ | exchange current density, A $m^{-2}$ |
| $i_s$ | electrode current density, A $m^{-2}$ |
| $j_i$ | mass flux, kg $s^{-1}$ $m^{-2}$ |
| $k$ | thermal conductivity, W $m^{-1}$ $K^{-1}$ |
| $K_{br}$ | permeability, $m^2$ |
| $l$ | entrance length, m |
| $n$ | surface normal |
| $n_m$ | number of participating electrons |
| $p$ | pressure, Pa |
| $Q$ | heat source/sink, W $m^{-3}$ |
| $Q_b$ | boundary heat source, W $m^{-2}$ |
| $Q_{br}$ | source term, kg $m^{-3}$ $s^{-1}$ |
| $R$ | universal gas constant; 8.314, J $mol^{-1}$ $K^{-1}$ |
| $T$ | temperature, K |
| $u$ | velocity field, m $s^{-1}$ |
| $v_{i,m}$ | stoichiometric coefficient |
| $\alpha_a$ | anodic transfer coefficient |
| $\alpha_c$ | cathodic transfer coefficient |
| $\beta_F$ | Forchheimer drag, kg $m^{-4}$ |
| $\varepsilon_p$ | porosity |
| $\eta$ | overpotential, V |
| $\mu$ | dynamic viscosity, Pa s |
| $\rho$ | density, kg $m^{-3}$ |
| $\sigma_l$ | electrolyte conductivity, S $m^{-1}$ |
| $\sigma_s$ | electrode conductivity, S $m^{-1}$ |
| $\phi_l$ | electrolyte potential, V |
| $\phi_s$ | electric potential, V |
| $\omega_i$ | mass fraction |

the electrolyte membrane. Without a major breakthrough in materials, increasing efficiency is required to push production of fuel cells.

Sasmito et al. have tried to improve thermal management in a PEMFC using a new flow reversal technique [2]. They proposed a novel design where there is a rapid reversal of the cooling air responsible for convective cooling. They developed a mathematical model which includes the fuel cell stack, the ambient environment, and the fan as its important parameters [2]. The model also takes into consideration various mass flow phenomena including heat transfer conditions, conditions of mass and momentum transfer, conservation of charge, Ohm's law applications, and the modeling of the fan. Thermal equilibrium and the electro-osmotic drag of water are some important assumptions made. The commercial software GAMBIT was used by the authors. They simulated the condition of flow reversal by having a different boundary condition from 'fan' to 'interior'. The results showed that a more uniform current density is achieved during fuel cell operation with the flow reversal concept. The water content in the membrane is more uniform when using the flow reversal concept. Also, the authors were able to show that increasing the rate of flow reversal results in a drop in uniformity of the current density [2].

Various designs and considerations for better and improved thermal management were studied by Sasmito, Birgersson, and Mujumdar [3]. Some of the considerations and techniques involved the forced convection, edge air cooling with help of fins, and forced and natural convection cooling. Mathematical modeling included a 1D, 2-phase flow model with the assumptions of electro-osmotic drag, mass, energy, and charge equilibrium [3]. The Butler–Volmer equation was used to study overpotential, primarily at the cathode. Considerations for thermal management include: (i) a closed manifold with liquid cooling applied at the top and bottom of the stack, (ii) a closed manifold with air cooling at the top and bottom of the stack, (iii) a closed manifold with air cooling applied to the edges, (iv) an open-cathode condition with fan-driven air convection, and (v) an open cathode stack with natural air convection cooling [3]. The authors were able to show that it is the liquid cooling which provides the most desirable results with respect to different types of thermal management techniques. Results also indicated that if the coolant rate of flow is increased, then there is an overall decrease in the stack average temperature; however, an increase in the coolant flow rate reduced the net power by up to 10%. The edge cooled stack design is lighter than the other air cooled designs. The authors concluded that the edge cooled stack has potential applications in the automotive sector. The authors also concluded that the coolant flow rate significantly modulates the output of the PEMFC [3].

Ashgari et al. worked on developing a comprehensive thermal management system for a 5 kW PEMFC system [4]. They performed both experimental studies and modeling analysis. The experimental study consisted of a single cell and a five cell stack with the same anode and cathode flow fields. Optimum operating conditions were found during the working of the cell [4]. The modeling analysis took into account the temperature distribution across the stack and the pressure drop across the flow field. Results indicated that there is a linear variation between the coolant flow rate and the pressure drop across the flow channels. Also, an increased coolant flow rate results in a uniform distribution of temperature and less parasitic losses [4].

A CFD study on the effect of straight and serpentine flow fields was performed by Hashemi and coworkers [5]. The researchers developed a comprehensive 3D model for this purpose taking into consideration non-isothermal phenomena to mimic reality. Some of the more important assumptions include a steady flow condition, a laminar flow regime, ideal gas behavior, and constant uniform activation overpotential. The authors started with the continuity equation in 3D and then applied it to obtain mass and momentum balance. Charge conservation was also considered [5]. The results showed that the concentration gradient is steeper at the membrane interface than at the center. Also the serpentine