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Thermal Characteristics of an Air-Cooled Open-Cathode PEM FC Stack via Numerical Investigation

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Abstract

In light of stricter emissions regulations and depleting fossil fuel reserves, Fuel Cell Vehicles (FCVs) are one of the leading alternatives for powering future vehicles. An open-cathode, air-cooled Proton Exchange Membrane Fuel Cell (PEMFC) stack provides a relatively simple electric generation system for a vehicle in terms of system complexity and number of components. The temperature within a PEMFC stack is critical to its level of performance and the electrochemical efficiency. Previously created computational models to study and predict the stack temperature have been limited by their scale and the inaccurate assumption that temperature is uniform throughout. The present work details the creation of a numerical model to study the temperature distribution of an 80-cell Ballard 1020ACS stack by simulating the cooling airflow across the stack. Using Computational Fluid Dynamics, a steady-state airflow simulation was performed using experimental data to form boundary conditions where possible. Additionally, a parametric study was performed to investigate the effect of the distance between the stack and cooling fan on stack performance. Model validation was performed against published results. The temperature distribution across the stack was identical for the central 70% of the cells, with eccentric temperatures observed at the stack extremities, while the difference between coolant and bipolar plate temperatures was approximately 10 °C at the cooling channel outlets. The results of the parametric study showed that the fan-stack distance has a negligible effect on stack performance. The assumptions regarding stack temperature uniformity and measurement were challenged. Lastly, the hypothesis regarding the negligible effect of fan-stack distance on stack performance was confirmed.

Keywords: *PEM fuel cells; Thermal management; Airflow simulation; Fuel Cell Vehicles; Coolant temperature; Stack temperature*

1. Introduction

In light of increasing levels of air pollution, as well diminishing global fossil fuel reserves, low-emission alternatives to the internal combustion engine (ICE) are being developed for future vehicles [1,2]. Electric vehicles (EVs) – both battery-based and hybrid variants – and hydrogen fuel cell vehicles (HFCVs) are the two leading alternatives to ICE vehicles [3–5]. The primary merit of these drivetrain systems is the significant reduction in greenhouse gas emissions relative to their conventional counterparts. The significance of this is evidenced by the negative environmental and health effects posed by the production and use of fossil fuels [6–8]. An advantage of HFCVs over battery-powered EVs is the longer vehicle range which is achieved due to higher energy density of compressed hydrogen [4,9,10]. This is particularly beneficial for passenger vehicles that operate in urban environments with increasingly strict emissions limits [11].

Within the field of hydrogen fuel cells, Proton Exchange Membrane Fuel Cells (PEMFCs) are already used for HFCVs [12]. The characteristic feature of PEMFCs is the hydrated membrane used to transport protons from the anode to the cathode. The dissociation of hydrogen at the anode and its subsequent reaction with oxygen at the cathode results in the flow of electric current which is used to power the vehicle. Electrochemical reactions within the cell produce heat as a by-product, due to a rise in entropy (ΔS), as given by the change in Gibbs free energy of the system (ΔG) [13,14]. The heat produced may be removed by dissipation to surroundings, unused reactants or air cooled PEM FC systems [14]. The air-cooled PEM systems are classified into two main categories: the active and the passive type [15, 16]. The main difference between these two approaches is the way that the air is introduced in the system. In the case where the reactant air (oxygen reduction reaction) and the air for cooling are supplied to the system separately via two different pathways, then the cooling is considered as active [17]. On the other hand, if the PEM FC system is based on natural convection of air with the external surface area of the stack, then the cooling is considered as passive [18]. Passive cooling refers to the use of conduction to dissipate heat; this is achieved using heat spreaders or heat pipes [19, 20]. Between those two configurations, the passive cooling approach is simpler, leading to a lower system cost, lower and easier maintenance and it can be applied also to lightweight applications, such as the utilisation of PEM FCs in UAVs [21]. Thus, the selection of the type of the cooling system depends mainly on the power grade of the PEM FC [22].

Most heat within the stack is removed by active cooling due to the low heat removal rate by the unused reactants and the low heat dissipation to the atmosphere [23, 24]. Removal of excess heat ensures that the stack operates at its optimum temperature, thus maximising its efficiency and lifespan [25, 26].

For stacks with power outputs below 10 kW, common cooling methods include air cooling, passive cooling, and liquid cooling [27, 28]. Liquid cooling is favourable relative to air cooling for high-power applications, when the stack power output exceeds 5 kW [25,27]. While liquid cooling results in a greater heat removal rate, the power required to operate ancillary components can counteract this gain [25]. Alternatively, an air-cooling system produces a smaller parasitic power loss, albeit with a lower cooling capacity. This procedure results in a simplified Balance of Plant (BOP) as well, which reduces the cost, complexity and weight of the cooling subsystem [29]. In such way, the oxidant and cooling subsystems are combined, as air provides the oxidant for electrochemical reaction at the cathode while also removing heat from the stack [29].

Primarily, the heat generation within a PEMFC stack is achieved by the electrochemical reactions and joule heating. Cumulatively, the total heat generation within the stack (Q_{gen}) can be approximated by [14]: $Q_{gen}=(1.2534-V_{cell})\cdot I\cdot n_{cell}$, where Q_{gen} *(W)* is the heat generated, V_{cell} *(V)* is the cell voltage, *I (A)* the stack current and n_{cell} the number of cells in stack.

Given that PEMFC stacks operate at temperatures in the range of 80 °C [30], it is safe to assume that heat dissipation via radiation is negligible [26,31]. The exit temperature of either the coolant or cathode reactant gas can be used to represent the stack temperature, although the actual stack temperature may be higher than the exit temperature [14].

An increase in stack temperature above the optimum value increases the cell potential by enhancing the kinetics of the electrochemical reactions [13,14,26]. However, prolonged operation at higher temperatures is likely to cause a drop in the FC stack power output [25]. Dehydration and subsequent thermal degradation of the membrane can occur at sustained periods of operation above the optimum temperature [26]. The membrane dehydration results in the increase of the ion transport resistance across the membrane, leading to Ohmic voltage losses [32, 33]. Alternatively, when the stack temperature is below the optimum value, cell potential decreases due to a drop in the rate of electrochemical reactions at both electrodes, also known as the 'activation polarisation' [13,14]. Additionally, the water vapour produced from the reduction of hydrogen at the cathode could condense within the channels at these temperatures, and could block the flow of reactants [14, 34]. This is referred to as 'flooding' and is highly detrimental to cell performance [26]. In addition to the maximum stack temperature, the temperature gradient within a PEM fuel cell has a profound effect on its performance [35]. Localised temperature deviations from the optimal value can impact transport phenomena at the reaction sites, resulting in a reduction of overall cell voltage [35, 36]. Thus, an uneven temperature distribution is intensified within a stack, where the free surface area of the cells is minimised.

With respect to modelling, there are primarily two methods employed to simulate a mixture of the main physical phenomena taking place in the PEM FC, such as the two phase reactant flow, electrochemical reactions, heat transfer, electron and proton transport, as well as the coolant flow [37]: the control method and the numerical method. The control method uses closed-loop control models to monitor and regulate a certain physical property within a desired range [38 - 40]. This strategy is relevant to the development of FC systems for electric vehicles [41]. A holistic approach to modelling facilitates optimisation of the cooling subsystem, which can help prolong the life of the FC system and improve performance [42, 43].

The numerical approach is used to model a mixture of physical phenomena and their variation across the FC. Simulation domains generally range in size from a channel to an entire stack [31,44]. However, the majority of studies based on numerical PEMFC models are limited in scale to the channel and cell-level [31, 45-47]. The complexity and the number of variables within a PEMFC stack necessitate smaller simulation domains in the interest of computational efficiency [37]. Recent numerical models include the creation of a model to predict the transport of water within a single cell [48], where the effects of water content on the electrochemical behaviour of the cell predicted accurately. A similar study [49] also incorporates the modelling of oxygen content and temperature. The effects of low humidity operating conditions with a thin MEA (Membrane Electrode Assembly) are elucidated by performing channel and cell-level simulations.

A relative subset of studies that utilise the numerical method employ computational fluid dynamics (CFD) to describe the fluid flow of the reactants and/or the coolant within a PEMFC

[21,34,35]. In a semi-empirical approach [31], a simulation of the coolant (air) flow and the introduction of the energy conservation equation within the bipolar plate, MEA and coolant domains produced results within 3% of experimental measurements. Simulations performed for a single channel and cell using a symmetry boundary condition to represent the rest of the FC stack.

On a similar approach [45], a purely analytical model was used to investigate the efficacy of different flow field designs within single cell. A variation of this approach is to couple the fluid flow, heat transfer, and electrochemical reactions, as presented by. [44]. An analytical model was created for a 5-cell stack, including the catalyst and gas diffusion layers. The results showed good correlation with experimental data. A simulation of major flow species and electrochemical effects within a single cell to study the effects of the cooling flow field orientation on temperature uniformity have been considered [46]. Two cooling flow field designs were studied: parallel and serpentine channels. The latter design showed a more uniform temperature distribution across the cell.

Most of the studies performed to date are limited in the size of the computational domain analysed. One of the largest scales of simulation is that of a 5-cell stack, which is deficient compared to 80-cell stacks observed in automotive applications [44]. The use of smaller computational domains warrants the use of symmetry or periodicity boundary conditions, with the assumption that the thermal characteristics of all cells within a stack are equivalent [31,46]. Another limitation is the use of idealised boundary conditions. An example of this is the application of a constant inlet air velocity for all channels within a cell [31]. This excludes other FC system components such as the cooling fan, housing, and inlet filter, and thus may not be representative of PEMFC operating conditions in practice.

In the current study, a numerical approach for analysing the cooling subsystem and the temperature distribution within a PEMFC stack is considered. The novelty of the current numerical approach is based on the scale of the computational domain. There is a significant increase in the size of the stack modelled relative to those seen previously, with all 80 cells being included [44]. By doing so, the temperature distribution across the entire stack is elucidated, which still remains unreported [37]. Moreover, the temperature results will test the validity of periodic/symmetry boundary conditions commonly utilised for cell-level simulations [31, 45, 46]. Their validity will be tested by examining the uniformity of temperature variation across all cells. Lastly, the proposed numerical model marks an advancement in PEMFC modelling by considering components within the broader FC system. Previous models employed idealised fluid flow boundary conditions, particularly those related to velocity and pressure [44, 45]. The model introduced in the present work utilises boundary conditions derived from data obtained experimentally, where possible. An example of this includes using OEM data to select the optimal cooling fan velocity. Further, the true nature of the coolant flow field near the stack is tested by producing a computational domain based on an existing FC system used in the real-world.

2. Methodology

2.1. Geometry

A dimensionally accurate 3D model of a PEMFC system was developed to provide an accurate baseline simulation. The geometry was based on an existing fuel cell system manufactured by Microcab Industries Ltd, Coventry, UK [50]. While all the components within the system were not essential for the simulation, they were added to investigate the effects of

the system layout on the thermal characteristics of the stack. The main components of the FC system model were:

- Ballard 1020ACS Fuel Cell Stack [51]
- FC Housing
  - Exterior panels
  - Stabilisers
  - Sealing foam
  - Intake filter
  - Mounts
- Fan
- Ancillary Components
  - Power wiring
  - Fasteners

Figure 1. Image of the FC system modelled (Ballard 1020ACS Stack model) in Figure 1a and 1b. The stack is presented in 1c and the partial view of the FC housing in Figure 1d.

The FC system, shown in **Error! Reference source not found.**, is centred on the Ballard 1020ACS fuel cell stack. The stack is encapsulated along 4 edges by foam, which forms a seal between the stack and housing, ensuring all air is directed through the stack [29]. The foam and stack are constrained within the housing by horizontal and vertical stabilisers, as shown in Figure 1c and 1d. Air is drawn into the stack using a fan that maintains a sub-atmospheric pressure within the housing. A filter on the other side of the stack protects it from atmospheric debris. By drawing air into the housing using negative pressure, air turbulence is reduced relative to pushing air via positive pressure [52]. On the housing exterior, mounts on either side provide a location to install the housing into the vehicle. Power wiring – connected to the stack electrodes – provides power to the vehicle via an electrical connector besides the mount.

2.2. Numerical Model

2.2.1. Assumptions

The following assumptions were made for the development of the numerical model:

- Incompressible, single-phase coolant (air) flow [31].
- Physical quantities – such as the bipolar plate (BP) temperature – remain constant across the height of a single cell [44].
- Perfect sealing between the foam and housing [29].
- Anode flow is neglected due to the low heat transfer rate (dead-ended) [31,43].
- Material properties are constant for the solid domains.
- Constant heat flux present across the active area of the MEA [31,45,47,53].
- Cell voltage is constant for all cells within the stack [31]
- Rotational effects of the fan are neglected.
- Fasteners and connecting rods were neglected in the computational domain [54].
- FC stack is generating the maximum rated power output [53].

- Coolant flow requirement exceeds the oxidant flow requirement, ensuring that the former governs the air flow rate through the FC system [53].

2.2.2. Computational Domain

In the interest of computational efficiency, 3 rows of air channels at the centre of the stack (240 channels) were simulated, which enabled a study into the thermal distribution across the stack (-y direction). The numerical model comprised of 3 physical domains:

- air
- bipolar plate (BP) (n = 80)
- MEA (n = 79)

Figurea presents the geometry used for the simulation. This was modelled by constructing a body bounded by the edge of the FC housing. Next, the solid domains being studied were subtracted from the fluid body using Boolean operations. In addition, Figure 2b restates the computational domain, along with the co-ordinate system used. The cells within the stack have been highlighted for clarity.

Figure 2. Figure 2a presents the computational domain used in the numerical model, while Figure 2b presents the computational domain with pertinent cells highlighted

2.2.3. Numerical Model and Modelled Phenomena

The oxidant, cooling and electrical subsystems were simulated together using the equations detailed below. The operating condition considered was that of steady-state operation of the FC stack at maximum nominal power. Thus, the highest heat generation rate was simulated, with the stack being subjected to the highest possible temperatures.

The airflow across the stack, which represents the oxidant and the cooling subsystems, was modelled using the k−ω turbulence model, where the turbulence is predicted Partial Differential Equations (PDE) for two variables (k and w). Fluid flow was assumed to be incompressible [31]. The model was selected due to flow separation that occurs at the channel exit points [54]. It uses the Reynolds Averaged Navier-Stokes (RANS) and the continuity equations to solve for the fluid velocity *u (m/s)* and pressure *p (Pa)*, as shown in Equations (1)-(3) [55, 56]:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \vec{v}) = 0 \tag{1}$$

where
- ρ fluid density [kg/m^3]
- t time coordinate [s]
- v velocity vector [m/s]

$$\frac{\partial \overline{u_\iota}}{\partial t} + \overline{u_\jmath}\frac{\partial \overline{u_\iota}}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \nu\frac{\partial^2 \overline{u_\iota}}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

where
- $\overline{u_\iota}$ components of averaged velocity vector
- t time coordinate [s]
- x_j component of coordinate vector
- $\bar{p}$ mean pressure [Pa]
- τ_{ij} component of Reynolds stress tensor

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \tag{3}$$

Additionally, the k-ω turbulence model solves for the eddy viscosity (μ_t), turbulence kinetic energy (k), and specific dissipation rate (ω) as shown in Equations (4)-(6) [57, 58].

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma_k \frac{\rho k}{\omega}\right)\frac{\partial k}{\partial x_j}\right] \tag{4}$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\gamma \omega}{k} P - \beta \rho \omega^2 + \frac{\partial}{\partial x_j}\left[\left(\mu + \sigma_\omega \frac{\rho k}{\omega}\right)\frac{\partial \omega}{\partial x_j}\right] \tag{5}$$

$$\mu_t = \frac{\rho k}{\omega} \tag{6}$$

where
- k — turbulence kinetic energy [m^2/s^2]
- B* — closure coefficient in turbulence-kinetic energy equation
- ω — specific dissipation rate
- σ, β — closure coefficients in the specific dissipation-rate equation

The formation of liquid water in the cathode channels (flooding) was neglected due to the optimum operating conditions assumed. Further, the equation for heat generation has been formulated under the assumption that all water produced in the stack leaves the system in the form of vapour [14]. Thus, the cooling effect of evaporation has been incorporated intrinsically into the model [31]. Consequently, single-phase fluid flow has been modelled in the interest of computational efficiency. This does not detract from the thermal performance of the stack. The energy equation used within the fluid domain is Equation (7) [55].

$$\frac{\partial \rho e}{\partial t} + \nabla(\rho e v) = -p \nabla v + \phi + k \nabla^2 T \tag{7}$$

where
- p — fluid pressure [Pa]
- Φ — viscous dissipation
- T — fluid temperature [K]
- e — specific internal energy [J/kg]
- ρ — fluid density [kg/m^3]
- v — fluid velocity [m/s]
- k_{th} — thermal conductivity [W/mK]

The electrical subsystem (electrochemical reactions) was decoupled from the model to investigate the cooling subsystem with more rigour. This was performed to improve the computational efficiency without detracting from its validity, as performed in previous studies [45, 47]. Thus, the reaction effect is represented by the term of heat generation (q_{gen}) at the MEA of each cell.

2.2.4. Materials

Default material properties for air (from COMSOL Multiphysics 5.3) were applied to the fluid domain. For the BP domain, material properties for 'Graphite 7087' were used. However, the value of thermal conductivity (k_{BP}) was set to 60 W/mK, which was obtained from the in-plane BP thermal conductivity used by Shahsavari *et al.* [31]. For the MEA domain, material properties for Nafion [14] were derived from published density values [46], thermal conductivity [59], and specific heat capacity [60].

2.2.5. Boundary Conditions

Periodicity boundary conditions were applied on the upper and lower surfaces (in the -xy plane) of all domains, as shown in Figure 3. This represented the computational domain as a repeated part of the entire FC stack [61].

Figure 3. Summary of boundary conditions applied: periodicity (purple); no-slip (green); heat flux (red).

The heat generation rate within a cell was determined using Equation (8). The cell voltage and stack current were determined from the polarisation curve published by Ballard Power Systems [53]. When operating at the maximum permissible stack current, the heat generation rate within a cell was 46.7 W, as shown in Equation (8).

$$\begin{aligned} Q_{cell} &= (1.253 - V_{cell}) \times I_{stack} \\ &= (1.254 - 0.63) \times 75.0 \\ \therefore Q_{cell} &= \ 46.7\ W \end{aligned} \tag{8}$$

The heat generation flux (q_{cell}) was thus calculated by dividing the heat generation rate by the active area of the cell, as shown in Equation (9). The active area of the cell (137.9 cm^2) was measured as the area of the MEA exposed to air within the cathode channels.

$$q_{cell} = \frac{Q_{cell}}{A_{active}} = \frac{46.7\ [W]}{0.01379\ [m^2]} = 3387\ [W/m^2] \tag{9}$$

where A_{active} cell active area [m^2]

Due to the modelling of the MEAs as 3D layers with finite thicknesses, the heat generation flux (q_{cell}) was reduced by half and applied to both sides of each MEA. Hence, the total heat generation from each cell was 46.7 W.

The surface highlighted in Figure 2 was set as the inlet of the fluid domain. To model the porous intake filter that is positioned at the inlet of the housing, the 'Grille' boundary condition was utilised. The quadratic loss coefficient (qlc) was derived from OEM data provided by ITG Air Filters [62]. The pressure drop (ΔP) across the filter as a function of inlet air velocity (v_{inlet}) is given in Equation (10). Neglecting the linear term, qlc was obtained from the coefficient of the quadratic term (28.215 kg/m^7). For air entering the housing, the ambient temperature T_{amb} of air was set to 20 °C.

$$\Delta P = 0.064 v_{inlet} + 28.215 v_{inlet}^2 \tag{10}$$

The fan was modelled by specifying the required air velocity to adequately cool the stack. This was derived from the coolant mass flow rate required to maintain the stack at its optimum

temperature [53]. Firstly, the optimum stack temperature (T_{opt}) was determined using Equation (11) [53]. The required coolant mass flow rate was then determined using Equation (12) [53]. The coolant heat removal rate ($Q_{removed}$) represents the total heat generation within the stack, which is given by $Q_{cell} \times n_{cell}$. Lastly, the required air velocity was calculated using Equation (13). Assuming the air density (ρ_{air}) to be 1.02 kg/m^3 [63], the outlet air velocity (v_{fan}) was determined to be 1.234 m/s.

$$T_{opt} = 0.53 I_{stack} + 26.01 = (0.53 \times 75.0) + 26.01 = 65.8\,°C \tag{11}$$

$$\dot{m}_{coolant} = \frac{Q_{removed}}{C_P \times (T_{stack} - T_{amb} - 0.403 Q_{removed})} \tag{12}$$

$$\dot{m}_{coolant} = \frac{46.7 \times 80}{1006 \times (65.8 - 20 - (0.403 \times 46.7))} = 0.138 \frac{kg}{s}$$

where
$\dot{m}_{coolant}$	coolant mass flow rate [kg/s]
$Q_{removed}$	coolant heat removal rate [W]
C_P	coolant specific heat capacity [J/kgK]
T_{stack}	stack temperature (optimum) [°C]
T_{amb}	ambient air temperature [°C]

$$\dot{m}_{coolant} = \rho \cdot A_{fan} \cdot v_{fan} \left[\frac{kg}{s}\right] \tag{13}$$

where
A_{fan}	effective area of fan [m^2]
v_{fan}	outlet air velocity [m/s]

Lastly, the no-slip condition (u=0) was applied on the FC housing walls and all exterior surfaces of the FC stack. A summary of all pertinent boundary conditions is presented in Figure 3.

2.2.6. Solution

A computational grid consisting of 823,374 elements was created, with adequate resolution of the fluid flow boundary layers in the cathode channels [57]. A converged solution was obtained upon reduction of residuals to the order of 10^{-3} [57].

2.3. Parametric Study

The parameter investigated is the effect of the distance between the stack and the fan on the system's performance. There are very limited sources in literature regarding the packaging of PEMFC stacks, particularly air-cooled and/or open-cathode stacks. De las Heras *et al*. [29] remarked that the variation of the fan-stack distance (20-30 cm) had no practical effects on performance of the PEMFC stack. This claim is investigated over a larger range of distances in this work. A range of 6 values were chosen based on the diameter of the fan (D_{fan} = 400 mm), as shown in Table 1. Fan-stack distance is highlighted within the computational domain in Figure 2a.

Table 1. Values of fan-stack distances considered for the parametric study

2.4. Validation of Numerical Model

Validation of the numerical model was performed using experimental data by Shahsavari *et al.* [31] where the Ballard ACS stack was operated at conditions that generate the maximum amount of heat, identical to those modelled in this work. The experimental measurements were taken at a location 40% along the height of the cell, located at the middle of the stack. Thus, the simulation measurements were taken at the central cell (#41) to enable consistency between data sets. While this does not entirely align with the distance used in this study (50%), measurements taken at 40% and 50% are nearly identical [44].

For the validation process, temperature measurements of the bipolar plate at 4 points across the cell width were compared. The comparison is presented in Figure 4a. The four experimental measurements (highlighted in purple) at points $y_1 - y_4$ were taken at points across the width of that cell and are presented in Figure 4b [31].

The maximum discrepancy between the data sets is 9.4% and is observed near the inlet of the channel. In this region, the model underestimates the experimental measured stack temperature by approximately 6 °C. The discrepancy between datasets falls near the channel outlet; the maximum stack temperature in the simulation differs by 3.3%. Given that the maximum stack temperature is a significant characteristic of FC performance, the level of agreement observed between data sets at higher temperatures proves the validity of the model. Figure 4c shows the comparison on the temperature for the points compared and at the same time shows the deviation at each point.

Figure 4. Comparison of experimental temperature measurements. Figure 5b represents the experimental data by [31] and the plot at Figure 5a the numerical data from the current study. Fig. 5c, shows the direct comparison between the experimental and the numerical data (left) and the relative difference (right).

3. Results and Discussion

3.1. Baseline Simulation

Error! Reference source not found. 5a shows the temperature distribution across the FC stack, as illustrated on a cut (-xy) plane that intersects only the BP and MEA domains. At the centre of the stack, the temperature along the -x direction increases across the cell. A change from 58 °C to approximately 72 °C is observed, representing a rise of 14 °C (24%).

Error! Reference source not found. 5b shows the BP temperature variation from the stack inlet to stack outlet face (-x direction) for 5 cells. Cells adjacent to the channels stated (#2, #20, #41, #60 and #79) were analysed. Cell temperature variation is consistent for approximately 70% of cells in the middle of the stack. This is indicated by the coincidence of plots for cells 20, 41 and 60 as illustrated in detail at the inlaid in **Error! Reference source not found.** 5b. Temperature across the rest 30% of cells (at either ends) is marginally lower as also seen in the inlaid. At a given position in the -x direction, cell temperature is approximately 5 °C lower at peripheral cells. For example, by comparing cell #2 and #41, a difference of 6 °C (8.5%) is observed close to the channel outlet. A minor difference of approximately 1 °C is noted between the temperature of cells #2 and #79. This asymmetry across the stack can be attributed to the computational accuracy of the solver used. An increase in the air temperature is observed across the stack due to the heat transfer from the surrounding BP and MEA layers via convection. It is noted that the temperature variation is nearly similar for the 3 rows of cooling channels. Figure 5c presents the temperature variation across the BP and air channel within cell # 41 viewed in the -xz plane. The magnitude of temperature increase in air along the channels is higher relative to that observed in the BP. For the central channel in the stack (#41), air

temperature at the geometric centre increases from 20 °C (ambient) to approximately 62 °C. This represents an increase of approximately 208%.

Figure 5. Temperature distribution within the BP and MEA domains (-xy plane) (5a). Figure 5b shows the temperature plot within the BP domain for 5 different cells and Figure 6c presents the temperature variation across the BP and air channel within cell # 41 viewed in the -xz plane

Figure 6 depicts the air temperature variation across the FC system for the 5 studied channels from the centre row (geometric centre). A gradual increase is observed along the cells, while steep increases are seen at the stack inlet and outlet. While the overall trend is consistent for all cells, there is a temperature difference of approximately 4 °C between cell #41 and cell #2. This represents a difference of 6.9% relative to the temperature at cell #2.

Figure 6. Plot of temperature within the air domain for 5 cathode cells *Cell #2, Cell #20, Cell #41, Cell #60 and Cell #79)*

A comparison between the air and BP temperature variation across cell #41 is presented in Figure 7. The air temperature plotted was the average temperature over a cross-section of the channel and is not the temperature at the geometric centre. This was done to account for the existence of the thermal boundary layer within the channel. It is observed that the air experiences a greater relative increase in temperature (123%) across the channel as compared to the bipolar plate (22%). Notably, there exists a temperature difference of approximately 12 °C at the channel outlet (X*=1) between the air and bipolar plate.

Figure 7. Plot of (average) cathode air and BP temperature across cell #41

The results obtained provide a clearer and deeper understanding of the temperature distribution across the entire FC system, representing an advancement of progress in PEMFC coolant modelling [31,37,45-47]. The temperature distribution obtained across the stack challenges the assumptions previously made in similar studies. The temperature variation within each cell is not identical across the stack. While the temperature variation within a cell is approximately identical from cells #11 to #70, a significant variation is observed at the ends of the stack. A minimum temperature of 50.14°C is observed in cells #1 and #80. This outcome suggests that there is a risk of flooding in the cathode channels in the cells at stack extremities [14,26]. Thus, the results dispute the assumptions made in literature regarding the identical temperature expected in each cell, reflected by the use of symmetry boundary conditions [43, 46].

For a given cell, a significant difference in temperature variation within the air and BP domains is observed. The difference of approximately 10 °C challenges the convention of using the coolant outlet temperature as a 'good approximation' of stack temperature [14]. This convention, when applied to an air-cooled, open cathode PEMFC stack, could potentially underestimate the stack temperature by approximately 17%. This could result in an enhanced level of electrochemical reactions, increasing the rate of energy and heat generation. If prolonged, this would cause thermal degradation and irreversible damage to the stack.

Figure 8 illustrates the streamlines of airflow across the FC system. The use of negative pressure to draw air into the housing through the inlet filter (bottom) facilitates laminar flow through the majority of the system's regions. A large proportion of flow from the stack exits the housing uninterrupted. An exception to this is the flow exiting from the central cells, behind

the cooling fan hub. Air from these cells stagnates as it reaches the hub before being drawn out by the fan. Furthermore, vortices are observed in the regions between the foam and housing walls at the corners. However, as shown in Figure 8, the vortices are nearly stagnant ($v \approx 0$) and thus do not affect the adjacent flow of air.

Figure 8. Plot of streamlines across the FC system (-xy plane)

Figure 9a illustrates the air velocity across the FC system. The velocity of air entering the stack (hereafter referred to as the *'primary flow'*) is approximately 0.60 m/s in the central region of the stack. Close to the edges of the stack, the velocity is 0.50 m/s near the transitional region between the vortices and the primary flow. Due to the constriction in flow cross-sectional area as air enters the channels, it accelerates rapidly to a maximum value of 5 m/s. Subsequently, as the air leaves the channels and expands into the housing region, the flow decelerates to a velocity similar to that observed at the housing inlet. The development of flow in the central channel is also explained in Figure 9b.

Figure 9. Plot of air velocity [m/s] across the (a) FC system (-xy plane) (b) cathode channels of cell #41 (-xz plane)

Close to the fan, flow accelerates to a maximum value of 1.23 m/s, equal to the velocity defined at the outlet boundary. Behind the fan hub and at the corners of the housing, the flow is nearly stationary. This is verified by a plot of channel velocities for 5 cells across the stack, as seen in Figure 10. Air crossing channel #20 and #60 are accelerated due to their position behind the active area of the fan. Conversely, air exiting the other channels stagnates at the fan hub or housing walls.

Figure 10. Plot of air velocity [m/s] within cathode channels for 5 cells (Cell #2, Cell #20, Cell #41, Cell #60 and Cell #79)

The pressure within a large proportion of the FC system is below the atmospheric level, which is expected because of the negative pressure air cooling system. Figure 11 shows the pressure distribution across the system. The static pressure after the porous inlet filter is -0.06 Pa up to the stack. Upon entering the channels, air pressure drops due to the rapid acceleration described in Figure 9. The pressure falls to -12 Pa at a rate of 5.21 Pa/mm within the first 10 mm of the channels. Thereafter, pressure falls at an approximately constant rate of 0.33 Pa/mm until the end of the channel. The lowest pressure reached within the channels is -35 Pa before the air expands into the housing. A rise of approximately 2 Pa is observed during this expansion; air pressure remains relatively constant until the exit of the housing.

Figure 11. Plot of air pressure [Pa] across the FC system (-xy plane)

Moreover, Figure 12 shows the variation in the air pressure across the 5 representative cathode channels. Like the trend observed for velocity, air flowing through channels behind the fan active area experiences a continual fall in pressure. Conversely, air incident upon the fan hub and housing walls stagnates, experiencing a minuscule rise in pressure of approximately 0.7 Pa.

Figure 12. Air pressure [Pa] within cathode channels for 5 cells (Cell #2, Cell #20, Cell #41, Cell #60 and Cell #79)

Turbulent kinetic energy (k) was analysed within the fluid domain to identify the areas of turbulence. Figure 13 depicts the turbulent kinetic energy with streamlines superimposed. Air flow is relatively laminar in the region of the housing after the stack. Within the inlet region of the housing, k reaches a maximum value of 0.01 m^2/s^2, which is observed close to the corners of the vertical foam ahead of the stack. Despite the presence of eddies in the upper region of Figure 13, these do not produce turbulence due to the flow being nearly stationary in this region, as also have been discussed at Figure 8.

Figure 13. Plot of turbulent kinetic energy [m^2/s^2] across the FC system (-xy plane)

The velocity and turbulent kinetic energy fields obtained from the previous analysis, strengthen the hypothesis that negative pressure promotes even air flow across the stack [42]. As evidenced by Figure 9, the velocity, and thus the coolant mass flow rate, was nearly constant across all cooling channels within the stack. Furthermore, the presence of a streamline in each cooling channel demonstrates the existence of an even flow field across all cells in the stack. Additionally, the minimal levels of turbulence observed were confirmed by Figure 13.

Primarily, the validity of results obtained was limited by the size of the computational domain. The use of periodicity could not accurately predict the temperature or pressure at the corners of the stack, for example. The eccentric temperatures observed at the end of the stack would likely be observed at other extremities of the stack. Nevertheless, the results presented are a novel reflection of the real-world operating conditions within a PEMFC stack.

3.2. Parametric Study

As mentioned previously, the parametric study considers 6 fan-stack distances: 40 mm, 100 mm, 200 mm, 300 mm, 400 mm and 800 mm corresponding to 10, 25, 50, 75, 100 and 200% of the fan diameter (D). Figure 14 depicts the temperature variation across the central cell (cell *#41*) for each of the cases studied. As evidenced by the coincidence of nearly all the lines, the distance between the stack and fan had no discernible effect on the stack temperature variation. One exception was the smallest distance considered (40 mm; 10% D_{fan}) as highlighted on the inlaid at Figure 14. Across the width of the cell, the BP temperature was approximately 2.5% higher relative to the baseline simulation.

Figure 14. Plot of BP temperature across cell #41 for each fan-stack distance considered

In addition, Figure 15 illustrates the air temperature variation for cell #41 across the FC system, with the x-axis normalised between a value of 0 and 1 (X^*). All cases considered exhibit a relative similar trend in the temperature increase, as air flows through the cooling channel. For a fan-stack distance of 40 mm (10% D_{fan}), terminal air temperature as it leaves the housing is 2.6% higher than that for the baseline simulation. Conversely, for a fan-stack distance of 800 mm (200% D_{fan}), the temperature is 1.6% lower than the baseline simulation.

Figure 15. Plot of cathode channel temperature across cell #41 for each fan-stack distance considered

Figure 16 presents the variation in velocity magnitude along channel #41 for each of the cases of fan-stack distance considered. At the housing inlet and near the housing exit, there is a minimal difference between velocities for all fan-stack distances. Within the stack, the highest difference relative to the baseline simulation is exhibited by D_{fan} = 40 mm; in this region the maximum velocity is 4.2% lower (4.6 m/s) than the baseline simulation (4.8 m/s).

Figure 16. Plot of air velocity across cell #41 for each fan-stack distance considered

Moreover, Figure 17 depicts the variation in pressure along channel #41 for each of the cases considered. Similar to the trend observed for temperature and velocity, there is no discernible variation in pressure with fan-stack distance. However, there exists a minimal increase in pressure of 6.8% for D_{fan}=40 mm relative to the baseline simulation. This is observed after the stack outlet within the housing.

Figure 17. Plot of air pressure across cell #41 for each fan-stack distance considered

The results obtained pertaining to the variation in fan-stack distance were relatively similar for all cases simulated. The effects of the FC system on stack performance have not been extensively studied. These results prove that the distance between the stack and the fan has no discernible effect on its performance [29]. However, from the results presented, it is evident that a distance of at least 10% of the fan diameter is required to ensure adequate airflow to the cooling channels directly behind the cooling fan hub. This is also necessary to accommodate electrical components, such as the connectors and power wiring.

4. Conclusion

In the work presented, a numerical approach was introduced and utilised to analyse the thermal characteristics of an air-cooled open-cathode PEM FC stack. The study aimed to simulate the cooling airflow across a PEMFC stack and analyse the resultant temperature distribution. Based on a quantitative analysis of simulation results, it can be concluded that for an 80-cell stack, the temperature distribution is not identical within each cell. The results showed a variation within the cell temperature at the stack extremities. A significant variation between the air and BP temperature at cooling channel outlets was identified, suggesting that coolant outlet temperature is not an accurate measure of stack temperature. Lastly, the distance between the stack and fan in a negative pressure air cooling system has a negligible effect on stack performance. However, a distance of at least 10% of the cooling fan diameter is highly recommended.

The methodology employed in this study, particularly the use of a semi-empirical model using data from component manufacturers, has proven to be a valid representation of a PEMFC system when operating at maximum power. This numerical model elucidates the thermal characteristics across the stack for three rows of cooling channels. Further work in this area on a larger scale will further help understand the stack temperature at areas furthest from the fan centre.

To further elucidate the temperature distribution within a PEMFC stack, subsequent studies are required in this subject area. This may be performed by increasing the size of the computational domain, for example by including more channels.

It is intended that the findings of this study will aid those packaging PEMFC stacks, particularly for use in automotive vehicles. By performing a computational study into the effects of packaging on the FC stack performance, the guidelines outlined in this chapter should aid those making decisions regarding the placement of the stack within the entire drivetrain system.

In conclusion, this study bridges a long-standing gap in the subject area by quantifying the performance of a PEMFC stack in three dimensions. Moreover, the entire FC system has been taken into consideration using experimental data to formulate the computational model. Thus, the findings in this study challenge assumptions made in literature regarding the convention for measuring stack temperature, and the uniformity of stack temperature itself.

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