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PERFORMANCE ENHANCEMENT IN PROTON EXCHANGE MEMBRANE FUEL CELL - NUMERICAL MODELING AND OPTIMISATION

by

Surajudeen Olanrewaju Obayopo

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Supervisor: Prof. T. Bello-Ochende
Co-Supervisor: Prof. J.P. Meyer

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ABSTRACT

TITLE:	**PERFORMANCE ENHANCEMENT IN PROTON EXCHANGE MEMBRANE FUEL CELL - NUMERICAL MODELING AND OPTIMISATION**
AUTHOR:	**S.O. Obayopo**
SUPERVISOR:	**Prof. T. Bello-Ochende**
CO-SUPERVISOR:	**Prof. J.P. Meyer**
DEPARTMENT:	**Mechanical and Aeronautical Engineering**
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Sustainable growth and development in a society requires energy supply that is efficient, affordable, readily available and, in the long term, sustainable without causing negative societal impacts, such as environmental pollution and its attendant consequences. In this respect, proton exchange membrane (PEM) fuel cells offer a promising alternative to existing conventional fossil fuel sources for transport and stationary applications due to its high efficiency, low-temperature operation, high power density, fast start-up and its portability for mobile applications. However, to fully harness the potential of PEM fuel cells, there is a need for improvement in the operational performance, durability and reliability during usage. There is also a need to reduce the cost of production to achieve commercialisation and thus compete with existing energy sources. The present study has therefore focused on developing novel approaches aimed at improving output performance for this class of fuel cell.

In this study, an innovative combined numerical computation and optimisation techniques, which could serve as alternative to the laborious and time-consuming trial-and-error approach to fuel cell design, is presented. In this novel approach, the limitation to the optimal design of a fuel cell was overcome by the search algorithm (Dynamic-Q) which is robust at finding optimal design parameters. The methodology involves integrating the computational fluid dynamics equations with a gradient-based optimiser (Dynamic-Q) which uses the successive objective and constraint function approximations to obtain the optimum design parameters. Specifically, using this methodology, we optimised the PEM fuel cell internal structures, such as the gas channels, gas diffusion layer (GDL) - relative thickness and porosity - and reactant gas transport, with the aim of maximising the net power output. Thermal-cooling modelling technique was also conducted to maximise the system performance at elevated working temperatures.

The study started with a steady-state three-dimensional computational model to study the performance of a single channel proton exchange membrane fuel cell under varying operating conditions and combined effect of these operating conditions was also investigated. From the results, temperature, gas diffusion layer porosity, cathode gas mass flow rate and species flow orientation significantly affect the performance of the fuel cell. The effect of the operating and design parameters on PEM fuel cell performance is also more dominant at low operating cell voltages than at higher operating fuel cell voltages. In addition, this study establishes the need to match the PEM fuel cell parameters such as porosity, species reactant mass flow rates and fuel gas channels geometry in the system design for maximum power output.

This study also presents a novel design, using pin fins, to enhance the performance of the PEM fuel cell through optimised reactant gas transport at a reduced pumping power requirement for the reactant gases. The results obtained indicated that the flow

Reynolds number had a significant effect on the flow field and the diffusion of the reactant gas through the GDL medium. In addition, an enhanced fuel cell performance was achieved using pin fins in a fuel cell gas channel, which ensured high performance and low fuel channel pressure drop of the fuel cell system. It should be noted that this study is the first attempt at enhancing the oxygen mass transfer through the PEM fuel cell GDL at reduced pressure drop, using pin fin.

Finally, the impact of cooling channel geometric configuration (in combination with stoichiometry ratio, relative humidity and coolant Reynolds number) on effective thermal heat transfer and performance in the fuel cell system was investigated. This is with a view to determine effective thermal management designs for this class of fuel cell. Numerical results shows that operating parameters such as stoichiometry ratio, relative humidity and cooling channel aspect ratio have significant effect on fuel cell performance, primarily by determining the level of membrane dehydration of the PEM fuel cell. The result showed the possibility of operating a PEM fuel cell beyond the critical temperature ($\leq 80^{\circ}$C), using the combined optimised stoichiometry ratio, relative humidity and cooling channel geometry without the need for special temperature resistant materials for the PEM fuel cell which are very expensive.

In summary, the results from this study demonstrate the potential of optimisation technique in improving PEM fuel cell design. Overall, this study will add to the knowledge base needed to produce generic design information for fuel cell systems, which can be applied to better designs of fuel cell stacks.

Keywords: PEM fuel cell; Computational fluid dynamics; Optimisation algorithm; Design parameters; Reactant gas transport; Pin fin; Cooling channel; Higher temperatures; Optimal performance.

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PUBLICATIONS IN JOURNALS AND CONFERENCES

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Journal article submitted for publication

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NOMENCLATURE

A	Channel width (m)
$\boldsymbol{A}$	Hessian matrix of the objective function
A_{ch}	Cross-sectional area of channel (m^2)
A^c	Fin cross-sectional area (m^2)
B	Channel depth (m)
$\boldsymbol{B}_i$	Hessian matrix of the inequality function
c	Constant
a, b, c	Diagonals of Hessian matrices ***A, B, C***
$\boldsymbol{C}_j$	Hessian matrix of the equality function
C_F	Quadratic drag factor
C_p	Specific heat capacity (J kg^{-1})
c_r	Condensation rate constant
D	Gas diffusivity (m^2 s^{-1})
D_{ch}	Channel diameter (m)
D_f	Diameter of pin fin (m)
D_{eff}	Effective diffusivity (m^2 s^{-1})
D_h	Hydraulic diameter (m)
E	Electrolyte
E_{OCV}	Open-circuit voltage (V)
e^-	Electron
F	Faraday constant (96, 487 C mol^{-1})

F	Friction factor
$f(\mathbf{x})$	Objective function
$\tilde{f}(\mathbf{x})$	Objective approximate function
G	Computational domain width (m)
$g_j(\mathbf{x})$	j-th equality constraint function
$\tilde{g}_j(\mathbf{x})$	j-th inequality constraint approximate function
h	Enthalpy (J kg^{-1})
H	Computational domain height (m)
$h_k(\mathbf{x})$	k-th equality constraint function
$\tilde{h}_k(\mathbf{x})$	k-th equality constraint approximate function
h_{L}	Enthalpy of condensation/vaporisation of water (J kg^{-1})
I	Exchange current density (A m^{-2})
i_o	Local current density (Am^{-2})
j	Volumetric transfer current
k	Thermal conductivity (W m^{-1} K^{-1})
K	Permeability
L	Channel axial length (m)
MW	Molecular weight
M	Molar mass (g/mol)
$\dot{m}$	Channel mass flow rate (kg/s)
n	Electron number

n_d	Electro-osmotic drag coefficient
P	Pressure (Pa)
P^*	Wetted perimeter
P_c	Capillary pressure (Pa)
P_o	Poiseuille constant
P_{pump}	Pumping power (W)
$P[k]$	Successive sub-problem
Q	Volume flow rate (m^3/s)
r_p	Mean pore radius
r_w	Water condensation rate (s^{-1})
R	Universal gas constant (8.314 J mol^{-1} K^{-1})
Re	Reynolds number
R_f	Dimensionless flow resistance
R_{ohm}	Resistance of proton transfer through electrolyte membrane (Ωm^2)
RH	Relative humidity
S	Liquid saturation or source term
S	Pin spacing (m)
Sh	Sherwood number
S_h	Volumetric heat source term
s_w	Water saturation
$\mathbb{R}^n$	*n*-dimensional real space

T	Time (s)
T	Temperature (K)
U	Overall heat transfer coefficient
U_o	Average velocity at inlet (m/s)
U_0	Thermodynamic equilibrium potential
u, v	Velocities in the x- and y- directions (m/s)
$\mathbf{u}$	Velocity vector [ms^{-1}]
V	Volume (m^3)
V	Cell potential (V)
V_{avg}	Mass-averaged velocity (m/s)
V_d	Volume ratio in diffusion layer
V_s	Surface ratio in diffusion layer
x, y, z	Cartesian coordinate (m)
w	Water
w	Mean velocity (m/s)
W	Molar mass fraction of oxygen
V_w	Convective velocity
$\boldsymbol{x}^*$	Design variables
$\boldsymbol{x}^k$	Design points
j,k, m,n,r	Positive integer

Greek

Δ	Difference operator
β	Permeability (m^2)
ε	Porosity
υ	Viscosity of flow [kg m^{-1} s^{-1}]
μ	Fluid viscosity (kg m^{-1} s^{-1})
μ	Penalty parameter value
α_{an}	Electrical transfer coefficient (anode)
α_{cat}	Electrical transfer coefficient (cathode)
λ	Membrane water content
λ	Tip clearance ratio
V	Kinematic viscosity [m^2 s^{-1}]
κ	Ionic conductivity [S/m]
ζ	Pitch
φ	Solid fraction
η	Over-potential (V)
Φ	Phase potential function (V)
ρ	Density (kg m^{-3})
τ	Tortuosity
σ	Electrical conductivity

Subscripts

a	Air
an	Anode
avg	Average
c	Capillary
cat	Cathode
ch	Channel
D	Porous diffusion layer
e	Electrolyte
eff	Effective
f	Fuel
G	Gas
H	Hydraulic
k	species
L	Liquid water
m	Mass moment source
m	Membrane
max	Maximum
min	Minimum
opt	Optimum
px, *py*, *pz*	Momentum source terms

react	Electrochemical reaction
ref	Reference value
s	Electronic conductive solid matrix
sat	Saturation
T	Energy source term
w	Liquid water source
v	Vapor phase
x,y,z	Components in the *x*-, *y*- and *z*- directions

AC	Alternating current
BPP	Bipolar plate
BTU	British thermal unit
CESFF	Convection-enhanced serpentine flow field
CL	Catalyst layer
CO	Carbon monoxide
CO_2	Carbon dioxide
CFD	Computational fluid dynamics
CHP	Combined heat and power
DC	Direct current
EMF	Electromotive force
FEM	Finite element method
GDL	Gas diffusion layer

H_2	Hydrogen gas
HOR	Hydrogen oxidation reaction
HT	Higher temperature
ICE	Internal combustion engine
LFOPC	Leapfrog optimization program for constrained problems
MEA	Membrane electrode assembly
MFPM	Multi-facilitated proton membrane
NO_x	Nitrogen oxides
O_2	Oxygen
ORR	Oxygen reduction reaction
PEM	Proton exchange membrane
PEMFC	Proton exchange membrane fuel cells
Pt	Platinum
SQP	Sequential quadratic programming