

**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**

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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 ($\leq 80^{\circ}\text{C}$), 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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Papers in refereed conference proceedings

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2. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Thermodynamic Optimization of PEM Fuel Cell Stack Gas Channel for Optimal Thermal Performance. *Proceedings of the 14th International Heat Transfer Conference (ASME)*,

- IHTC-14, paper no. IHTC14-22233, Washington DC, USA, 8-13 August 2010.
3. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Numerical Study of effect of design and physical parameters on a PEM fuel cell performance. *Proceedings of the 8th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, HEFAT 2011, pp. 567, Pointe Aux Piments, Mauritius, 11-13 July 2011.
 4. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Optimising the Performance of a PEM Fuel Cell with Transverse Fins Insert in the Channel Flow using Mathematical Algorithm. *Proceedings of the ASME 2012 6th International Conference on Energy Sustainability & 10th Fuel Cell Science, Engineering and Technology Conference ESFuelCell2012*, San Diego, CA, USA, 23-26 July 2012.
 5. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Numerical Study and Optimisation of Channel Geometry and Gas Diffusion Layer of a PEM Fuel Cell. *Proceedings of the ASME 2012 6th International Conference on Energy Sustainability & 10th Fuel Cell Science, Engineering and Technology Conference ESFuelCell2012*, San Diego, CA, USA, 23-26 July 2012.
 6. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Impact of Cooling Channel Geometry on Thermal Management and Performance of a Proton Exchange Membrane Fuel Cell. *Proceedings of the 9th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, HEFAT 2012, Malta, 16-18 July 2012.

Papers in non-refereed conference proceedings

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2. S.O. Obayopo, T. Bello-Ochende, J.P. Meyer. Performance enhancement of PEM fuel cell through reactant gas channel and gas diffusion layer optimization. *Proceedings of the Second Postgraduate Renewable Energy Symposium*, NCRS2011, Paper no. NCRS010. pp. 1-15. Stellenbosch, South Africa, 17-18 November 2011.



TABLE OF CONTENTS

ABSTRACT	ii
ACKNOWLEDGEMENTS	v
PUBLICATIONS IN JOURNALS AND CONFERENCES	vii
TABLE OF CONTENTS	ix
LIST OF FIGURES	xiii
LIST OF TABLES	xvii
NOMENCLATURE	xviii
CHAPTER 1: INTRODUCTION	1
1.1 BACKGROUND AND MOTIVATION	1
1.2 REVIEW OF RELATED LITERATURE	7
1.2.1 OPTIMAL OPERATING CONDITIONS FOR PEM FUEL CELLS.....	8
1.2.2 FUEL GAS CHANNEL OPTIMISATION FOR PEM FUEL CELLS	16
1.2.3 REACTANT GAS TRANSPORT IN PEM FUEL CELLS.....	20
1.2.4 HEAT TRANSPORT AND COOLING IN PEM FUEL CELLS	25
1.3 JUSTIFICATION FOR THIS STUDY	28
1.4 RESEARCH OBJECTIVES	30
1.5 ORGANISATION OF THE THESIS	31
CHAPTER 2: FUNDAMENTALS OF PEM FUEL CELL SYSTEMS	33
2.1 INTRODUCTION	33
2.2 THE BASIC STRUCTURE OF A PROTON EXCHANGE MEMBRANE FUEL CELL.....	33
2.2.1 PROTON EXCHANGE MEMBRANE	36
2.2.2 CATALYST LAYERS	36
2.2.3 GAS DIFFUSION LAYERS	38
2.2.4 BIPOLAR PLATES	39
2.3 PEM FUEL CELL STACK DESIGN.....	40
2.3.1 HYDROGEN FUEL CELL SYSTEM COMPONENTS.....	42

2.4 THEORIES OF TRANSPORT AND ELECTROCHEMICAL PROCESSES IN PEMFC	45
2.4.1 CONSERVATION EQUATIONS.....	46
2.4.2 NUMERICAL MODELS OF INDIVIDUAL PEM FUEL CELL COMPONENTS.....	52
CONCLUSION.....	69
CHAPTER 3: NUMERICAL MODELLING FRAMEWORK.....	69
3.1 INTRODUCTION	69
3.2 NUMERICAL METHOD.....	69
3.2.1 NUMERICAL MODELLING PROCEDURES.....	70
3.3 NUMERICAL OPTIMISATION	72
3.3.1 CONSTRAINED OPTIMISATION.....	72
3.3.2 THE DYNAMIC-Q METHOD	73
3.3.3 DYNAMIC-Q APPROACH: CONSTRUCTING SPHERICAL QUADRATIC SUBPROBLEMS.....	75
3.3.4 THE OBJECTIVE AND CONSTRAINT FUNCTIONS GRADIENT APPROXIMATION.....	78
3.3.5 ADVANTAGE OF DYNAMIC-Q ALGORITHM.....	79
CONCLUSION.....	80
CHAPTER 4: NUMERICAL OPTIMISATION OF OPERATING AND DESIGN PARAMETERS FOR A PEM FUEL CELL	81
4.1 INTRODUCTION	81
4.2 MODEL DESCRIPTION	84
4.2.1 MODEL ASSUMPTIONS	88
4.2.2 GOVERNING TRANSPORT EQUATIONS	88
4.2.3 CHANNEL CROSS-SECTION.....	92
4.2.4 FLUID FLOW THROUGH GAS DIFFUSION LAYER.....	95
4.2.5 BOUNDARY CONDITIONS.....	96
4.2.6 SOLUTION TECHNIQUE.....	97
4.2.7 MODEL VALIDATION.....	98
4.3 MODEL RESULTS AND DISCUSSION.....	99

x

4.3.1 PRESSURE DROP IN FLOW CHANNEL.....	99
4.3.2 EFFECT OF PHYSICAL PARAMETERS ON PROTON EXCHANGE MEMBRANE FUEL CELL PERFORMANCE	100
4.3.3 EFFECT OF DESIGN PARAMETERS ON PROTON EXCHANGE MEMBRANE FUEL CELL PERFORMANCE	105
4.3.4 OPTIMAL CHANNEL GEOMETRY.....	109
CONCLUSION.....	114
CHAPTER 5: OPTIMISING REACTANT GAS TRANSPORT IN A PROTON EXCHANGE MEMBRANE FUEL CELL WITH A PIN FIN INSERT IN CHANNEL FLOW	116
5.1 INTRODUCTION	115
5.2 MODEL DESCRIPTION	119
5.2.1 GOVERNING EQUATIONS.....	121
5.2.2 NUMERICAL PROCEDURE	126
5.3 MATHEMATICAL OPTIMISATION ALGORITHM.....	127
5.4 OPTIMISATION PROBLEM FORMULATION	128
5.4.1 OPTIMISATION CONSTRAINTS.....	128
5.4.2 OPTIMISATON PROCEDURE	130
5.5 RESULTS AND DISCUSSION	132
5.5.1 RESULTS OF FLOW FIELD.....	132
5.5.2 RESULTS OF PIN FIN GEOMETRY.....	135
5.5.3 OPTIMISATION RESULTS.....	139
5.5.4 PERFORMANCE EVALUATION.....	143
CONCLUSION.....	146
CHAPTER 6: MODELLING AND OPTIMISATION OF COOLING CHANNEL GEOMETRIC CONFIGURATION FOR OPTIMAL THERMAL PERFORMANCE OF A PROTON EXCHANGE MEMBRANE FUEL CELL	147
6.1 INTRODUCTION	147
6.2 MODEL DESCRIPTION	152



6.2.1 BASIC ASSUMPTIONS	155
6.2.2 GOVERNING EQUATIONS	156
6.2.3 NUMERICAL PROCEDURE	159
6.3 MATHEMATICAL OPTIMISATION ALGORITHM.....	160
6.4 OPTIMISATION PROBLEM FORMULATION	161
6.4.1 DESIGN VARIABLE CONSTRAINTS	162
6.4.2 OPTIMISATION PROCEDURE.....	162
6.5 RESULTS AND DISCUSSION	164
6.5.1 MODEL VALIDATION.....	164
6.5.2 PARAMETRIC STUDY RESULTS.....	165
6.5.3 OPTIMISATION RESULTS	172
CONCLUSION.....	179
CHAPTER 7: CONCLUSIONS AND RECOMMENDATIONS	180
7.1 CONCLUSIONS.....	180
7.2 RECOMMENDATIONS	183
REFERENCES.....	186
APPENDICES.....	216

LIST OF FIGURES

Figure 1.1 Comparison between hydrogen and gasoline as energy currency on service delivery chain [10].....	3
Figure 2.1 Schematic diagram of a single PEM fuel cell.....	34
Figure 2.2 The basic structure of a PEM fuel cell showing the path of the electrochemical reaction [15].....	35
Figure 2.3 Fuel cell stack component [71].....	40
Figure 2.4 A schematic of a complete hydrogen-air fuel cell system [115].	43
Figure 4.1 Schematic diagram of a PEM fuel cell showing different zones and species transport across the zones. The net water flux is the sum of: (A ₁) electro-osmotic effect, (A ₂) diffusion effect and (A ₃) the permeability effect.....	85
Figure 4.2 The discretised three-dimensional computational domain of a single PEM fuel cell.....	86
Figure 4.3 Channel cross-sectional view.....	93
Figure 4.4 Comparison of numerical model prediction and experimental polarisation curves at base condition.	99
Figure 4.5 Pressure drop along the model flow channel at base operating conditions for a channel depth of 2.0 mm and width of 1.2 mm.....	100
Figure 4.6 Effect of temperature on cell performance at base conditions.	101
Figure 4.7 Effect of cathode gas flow rate on cell performance at base conditions..	102
Figure 4.8 Effect of gas diffusion layer porosity on cell performance at base conditions.....	103
Figure 4.9 Effect of operating pressure on cell performance at base conditions.....	104
Figure 4.10 Effect of cathode gas stoichiometry on cell performance at base conditions.....	105
Figure 4.11 The cell current density at different channel depths at a cell potential of 0.3 V, a temperature of 70°C and a mass flow rate of 5e-06 kg/s.....	106
Figure 4.12 The cell current density at different channel widths at a cell potential of 0.3 V and a temperature of 70°C.	107

Figure 4.13 The cell current density for counterflow orientation (2.61 A/cm^2) and co-flow orientation (2.54 A/cm^2) at base case conditions, for a channel depth of 2.0 mm and a channel width of 1.2 mm.....	108
Figure 4.14 Contours of mass fraction of hydrogen at the anode for (a.) counterflow and (b.) co-flow cases at the base case operating conditions.....	109
Figure 4.15 Effect of porosity and channel depth on the cell current density.	110
Figure 4.16 Optimum depths as a function of flow rate and gas diffusion layer porosity.	111
Figure 4.17 Effect of flow rate and gas diffusion layer porosity on the cell current density.....	112
Figure 4.18 Effect of porosity and channel width on the cell current density.....	112
Figure 4.19 Optimum widths as a function of flow rate and gas diffusion layer porosity.	113
Figure 5.1 PEMFC half-cell model with two transverse pin fins along the flow channel.....	120
Figure 5.2 The representative grid system and computational domain.	127
Figure 5.3 Optimisation automation flow diagram.....	131
Figure 5.4 Effect of Reynolds number on the flow field for different flow field configurations ($s/d = 5, \lambda = 0.2$): (a) $\text{Re} = 50$, (b) $\text{Re} = 150$, (c) $\text{Re} = 250$	133
Figure 5.5 Effect of Reynolds number on the flow field for different flow field configurations ($s/d = 5, \lambda = 0.6$): (a) $\text{Re} = 50$, (b) $\text{Re} = 150$, (c) $\text{Re} = 250$	134
Figure 5.6 Contours of tangential velocity for different flow field configurations ($s/d = 5, \lambda = 0.6$): (a) $\text{Re} = 50$, (b) $\text{Re} = 150$, (c) $\text{Re} = 250$	134
Figure 5.7 Fuel channel friction factor as a function of the Reynolds number and pitch at a clearance ratio, $\lambda = 0.3$	135
Figure 5.8 Fuel channel friction factor as a function of the Reynolds number and clearance ratio at a pitch, $s/d = 5$	136
Figure 5.9 Fuel channel friction factor as a function of the Reynolds number and GDL porosity at a pitch, $s/d = 5$, and a clearance ratio, $\lambda = 0.3$	137
Figure 5.10 Effect of optimised clearance ratio on the peak channel flow resistance... ..	138

Figure 5.11 Effect of optimised pitch on the channel peak fuel channel flow resistance.....	139
Figure 5.12 The minimised fuel channel flow resistance as a function of Reynolds number for a fixed GDL porosity, $\varepsilon = 0.5$, and a tip clearance ratio, $\lambda = 0.3$	140
Figure 5.13 Optimal clearance ratio as a function of Reynolds number at a fixed pitch, $s/d = 5$, and a GDL porosity, $\varepsilon = 0.5$	141
Figure 5.14 Optimal pitch as a function of Reynolds number at a fixed clearance ratio, $\lambda = 0.3$, and a GDL porosity, $\varepsilon = 0.5$	141
Figure 5.15 Effect of channel flow resistance on the optimised clearance ratio at a fixed pitch, $s/d = 5$, and a GDL porosity, $\varepsilon = 0.5$, at Reynolds number of 250.....	142
Figure 5.16 Effect of channel flow resistance on the optimised pitch at a fixed clearance ratio, $\lambda = 0.3$, and a GDL porosity, $\varepsilon = 0.5$, at a Reynolds number of 250.....	143
Figure 5.17 Fuel channel pressure drop as a function of the applied pressure drop for a channel with pin fin ($s/d = 5, \lambda = 0.3$) and one without pin fin.	144
Figure 5.18 Pumping power as a function of tip clearance ratio at a pitch, $s/d = 5$, and GDL porosity, $\varepsilon = 0.6$, at a Reynolds number of 250.....	145
Figure 6.1 A schematic diagram of a 3-D model of PEM fuel cell system with cooling channels embedded in the bipolar plates.....	153
Figure 6.2 The discretised three-dimensional computational domain of a single PEM fuel cell with cooling channels.....	160
Figure 6.3 Optimisation automation flow diagram.....	163
Figure 6.4 Comparison of numerical model prediction and experimental polarisation curves at base condition.	165
Figure 6.5 Effect of temperature on the PEM fuel cell performance at base conditions.....	166
Figure 6.6 The cell current density as a function of temperature and the operating cell voltage.....	167
Figure 6.7 $I-V$ curve at varying stoichiometry number. $P = 3.0$ bar and $Re = 500$...	168
Figure 6.8 Effect of stoichiometry ratio on the PEM cell temperature at cell voltage of 0.7 V.....	169

Figure 6.9 *I-V* curve at varying relative humidity (*RH*). $P = 3.0$ bar and $Re = 500$..170

Figure 6.10 The cell current density at different aspect ratio at a cell potential of 0.7 V and a fixed Reynolds number of 500.....171

Figure 6.11 Current density at three cases of channel aspect ratio and $Re = 500$172

Figure 6.12 Effect of optimised cooling channel aspect ratio on the peak fuel cell current density at different temperatures.....175

Figure 6.13 Effect of Reynolds number and temperature on the optimised aspect ratio of the cooling channel.....176

Figure 6.14 Effect of Reynolds number on the maximum current density at different cell temperatures.....177

Figure 6.15 The local distribution of temperature along the membrane at different cooling channel aspect ratios and cell operating voltage of 0.7 V and $Re = 500$: (a) $H/W = 1.875$, (b) $H/W = 2.500$ and (c) $H/W = 2.813$178



LIST OF TABLES

Table 1.1 Combustion properties of hydrogen compared with other fuels [4].....	4
Table 4.1 Base case geometric parameters of the modelled fuel cell.....	86
Table 4.2 Physicochemical properties of the modelled fuel cell	86
Table 5.1 Parameters of the modelled fuel cell.....	121
Table 6.1 Parameters and properties used in the present model.....	154
Table 6.2 The governing equation source terms in various regions of the fuel cell..	157
Table 6.3 Grid independence test.....	159
Table 6.4 Dimension of the cooling channels investigated for initial simulations....	161
Table 6.5 Values of optimised parameters.....	173
Table 6.6 Polarisation data at optimised conditions and varying cell operating temperatures at $Re = 500$	173



NOMENCLATURE

A	Channel width (m)
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)
B_i	Hessian matrix of the inequality function
c	Constant
a, b, c	Diagonals of Hessian matrices A, B, C
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 ($\text{W m}^{-1} \text{K}^{-1}$)
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
\square^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
\mathbf{x}^*	Design variables
\mathbf{x}^k	Design points
j, k, m, n, r	Positive integer

Greek

Δ	Difference operator
β	Permeability (m ²)
ε	Porosity
ν	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

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



<i>react</i>	Electrochemical reaction
<i>ref</i>	Reference value
<i>s</i>	Electronic conductive solid matrix
<i>sat</i>	Saturation
<i>T</i>	Energy source term
<i>w</i>	Liquid water source
<i>v</i>	Vapor phase
<i>x,y,z</i>	Components in the <i>x</i> -, <i>y</i> - and <i>z</i> - directions
<i>AC</i>	Alternating current
<i>BPP</i>	Bipolar plate
<i>BTU</i>	British thermal unit
<i>CESFF</i>	Convection-enhanced serpentine flow field
<i>CL</i>	Catalyst layer
<i>CO</i>	Carbon monoxide
<i>CO₂</i>	Carbon dioxide
<i>CFD</i>	Computational fluid dynamics
<i>CHP</i>	Combined heat and power
<i>DC</i>	Direct current
<i>EMF</i>	Electromotive force
<i>FEM</i>	Finite element method
<i>GDL</i>	Gas diffusion layer

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