MACHINE LEARNING MODELS FOR PREDICTIVE ANALYSIS OF PRESSURE DROP AND TEMPERATURE IN POLYMER ELECTROLYTE MEMBRANE FUEL CELL STACKS TO FIND OPTIMAL FABRICATION PARAMETERS

HANHEE LEE

ESROP GLOBAL

NATIONAL UNIVERSITY OF SINGAPORE

2024

Declaration

I hereby declare that the thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in this thesis.

This thesis has also not been submitted for any degree in any university previously

Hanhee Lee

August, 2024

Acknowledgements

I would like to express my sincere gratitude to Professor Erik Birgersson. Professor Birgersson has provided me with profound insights and knowledge on various topics, including polymer electrolyte membrane fuel cell stacks, machine learning, deep learning, and the use of COMSOL. He has also taught me how to effectively present to a scientific audience and the importance of learning independently. His enthusiasm and encouragement have made this journey a truly pleasant and enriching experience.

Abstract

Contents

List of Figures

List of Tables

0.1 List of Symbols

Name	Description	Unit
p	Pressure	Pa
$\mathbf{u}, \mathbf{U}$	Velocity	m/s
ρ	Density	kg/m^3
$\mathbf{I}$	Identity tensor	-
$\mathbf{K}$	Viscous stress tensor	-
$\mathbf{F}$	Volume force vector	-
μ	Dynamic viscosity	Pa·s
T	Temperature	K
$\mathbf{n}$	Unit vector normal to the given surface	-
$\mathbf{G}$	Reciprocal wall distance	-
C_p	Specific heat capacity	J/(kg·K)
$\mathbf{q}$	Heat flux vector	-
Q	Heat source	W/m^3
k	Thermal conductivity	W/(m·K)
R	Thermal resistance	$(m^2·K)/W$
d	Thin layer thickness	m
Δ	Delta	-
ℓ	Length/Distance	m
u^+	Tangential velocity in viscous units	-
σ_w	Smoothing parameter	-
Re	Reynolds number	-
q	Quadratic loss coefficient	-
ϵ_p	Porosity	-
κ	Permeability	m^2
β_F	Forchheimer coefficient	kg/m^4
Q_m	Mass source	$kg/(m^3·s)$

Table 1: Variable Descriptions and Units

Name	Description
0	Standard Conditions
n	Unit vector normal to the given surface
p	Point
ted	Thermoelastic damping
b	Boundary
d	Down side
s	Solid
u	Up side
ref	Reference
w	Wall
T	Turbulent
$exit$	Exit
pc	Pressure curve

Table 2: Subscript Descriptions

Name	Description
T	Transpose

Table 3: Superscript Descriptions

Chapter 1

Introduction

1.1 Fuel Cells

Chapter 2

Neural Networks

Chapter 3

Literature Review

Chapter 4

Materials and Methods

Header	Symbol	Explanation	Unit
		Input Parameters	
Q	Q	**Heat generation** influences membrane hydration and operational efficiency; critical to prevent membrane dry-out and maintain ion conductivity.	Wm^{-2}
Tamb	T_{amb}	**Ambient temperature of the air** sets baseline thermal conditions; higher temperatures boost performance to a limit before causing potential overheating.	$^{\circ}C$
Uin	U_{in}	**Airflow velocity** determines oxygen supply rate, essential for maintaining optimal reaction rates and power output.	m/s
Wcc	W_{cc}	**Cathode channel width** determines oxygen flow and diffusion rates to the cathode, crucial for optimizing reaction efficiency.	mm
Hcc	H_{cc}	**Cathode channel height** affects gas flow resistance and water removal, essential for maintaining membrane hydration and preventing flooding.	mm
Lcc	L_{cc}	**Cathode channel length** influences the residence time of reactants and products along the channel, impacting overall fuel cell efficiency.	mm
Wr	W_r	**Rib width** supports mechanical stability and maximizes the active area available for reactions, balancing structural support with performance.	mm
Hr	H_r	**Rib height** controls the depth of flow channels, enhancing reactant distribution and efficient water management within the stack.	mm
		Output Performance Metrics	
Tsta	T_{stack}	**Stack temperature** is crucial for optimal reaction rates, membrane hydration, and to prolong the lifespan.	$^{\circ}C$
Delp	Δp	**Pressure drop** indicates the system's resistance to reactant flow; minimizing pressure drop is essential to enhance efficiency and ensure uniform distribution.	Pa

Table 4.1: Detailed Explanation of Variables

Chapter 5

COMSOL Model

5.1 Model Assumptions

1. The airflow entering the channel is turbulent. The Reynolds number exceeds 2300 at an inlet velocity (U_{in}) of 0.3 m/s.

2. Portions of the fuel cell not part of the cathode flow field are impermeable to air. While carbon paper is porous, the in-plane pressure drop is much greater than that of the cathode flow field.

3. The cathode flow field channels are modeled with a uniform height. The average offset (0.025 mm) is negligible compared to the channel height (1 mm).

4. Cathode flow fields are modeled with straight edges and right-angle folds. The fold radius (0.05 mm) is small compared to the channel width (1 mm).

5. Conservation of mass and momentum of airflow is assumed to be valid when transitioning between open spaces and cathode channels.

6. A representative unit cell approximates the entire stack, excluding edge effects near the terminals. Airflow entering the unit cell is uniform and symmetrical.

7. Channels are identical throughout the stack, resulting in no pressure drop differences between channels.

8. The channels are fully dry without condensation. The oxidant stoichiometry exceeds 100, ensuring water vapor produced is absorbed by the airflow, negating the need for accounting water saturation.

9. The losses from the fuel cell operation are converted to heat.

5.2 Workflow - Pressure Drop

The following steps outline the workflow process for the unit cell simulations conducted in COMSOL:

1. **Selection of Laminar Flow Model:**
    - This model was chosen because the airflow within the channels is laminar and is the largest contributor to the pressure drop across the stack.
    - The laminar flow model allows for faster convergence and has been shown to be accurate when compared with experimental results.
2. **Construction of Unit Cell:**
    - The unit cell was constructed using blocks with dimensions defined by equations to accommodate dimensional changes in the channels.
3. **Meshing Strategy:**
    - A custom mesh was employed, focusing on the transition areas between inflow and outflow within the channels with a finer mesh.
    - A coarser mesh was used within the channel and the air space between inflow and outflow.
    - A mesh independence study was performed during the mesh fine-tuning. The results are shown in Figure ?.
    - The difference between the blue dash (custom meshing) and green dots (physics-based extra fine meshing) is less than 3%, thus the blue dash mesh was selected for its speed and accuracy.
4. **Parameter Sweep Function:**
    - The parameter sweep function was utilized to explore all possible combinations for each stack size.
5. **Exporting Simulation Data:**
    - The inputs and outputs of the simulations were exported from COMSOL for further analysis.

5.3 Workflow - Temperature Stack

The following steps outline the workflow process for the unit cell simulations conducted in COMSOL:

1. **Selection of Physics Models:**

- The unit cell simulations were done using laminar flow physics as well as heat transfer in laminar flow.
- The parameter sweep function was utilized to explore all possible combinations in the parameter space.
- This model was selected because the flow through the channel is laminar and the simulation focuses on heat transfer within the channels.

2. **Construction of Unit Cell:**
    - The unit cell was constructed using blocks with dimensions defined by equations to accommodate dimensional changes in the channels.
3. **Heat Generation Simulation:**
    - Heat generation was simulated as a boundary heat source placed at the cathode side of the membrane.
4. **Heat Conduction Values:**
    - The heat conduction values for each layer in the fuel cell were obtained from various papers, as shown in Table 8-1.
5. **Meshing Strategy:**
    - A mesh independence study was conducted during the fine-tuning of the mesh. The results are shown in Figure ?.
    - The difference between the blue dash and green dots is less than 1.06%, hence the blue dash mesh was selected for its speed and accuracy.
6. **Exporting Simulation Data:**
    - The inputs and outputs of the simulations were exported from COMSOL for further analysis.

5.4 Parameters

Name	Value	Unit
Cell Area	0.005	m^2
Cell Voltage	0.6	V
Compression	0.1	-
Current	40	A
Hbp	5×10^{-5}	m
Hcc	1.25×10^{-3}	m
Hcp	3.15×10^{-4}	m
Hmem	1.5×10^{-5}	m
Kcp	1.5	$W\cdot m^{-1}K^{-1}$
Kmem	0.1	$W\cdot m^{-1}K^{-1}$
Lcc	0.03	m
pRef	1.0133×10^{5}	Pa
Q	5040	$W\cdot m^{-2}$
Tamb	293.15	K
Test	25.2	W
Uin	7.75	$m\cdot s^{-1}$
Wcc	0.001	m
Wr	5×10^{-5}	m

Table 5.1: Parameter Values

5.5 Materials

Name	Unit
Air	
Dynamic viscosity	$\mathrm{Pa} \cdot \mathrm{s}$
Ratio of specific heats	-
Heat capacity at constant pressure	$\mathrm{J}/(\mathrm{kg} \cdot \mathrm{K})$
Density	kg/m^3
Thermal conductivity	$\mathrm{W}/(\mathrm{m} \cdot \mathrm{K})$
Carbon Paper	
Density	kg/m^3
Heat capacity at constant pressure	$\mathrm{J}/(\mathrm{kg} \cdot \mathrm{K})$
Thermal conductivity	$\mathrm{W}/(\mathrm{m} \cdot \mathrm{K})$
Membrane	
Thermal conductivity	$\mathrm{W}/(\mathrm{m} \cdot \mathrm{K})$
Steel Grade 316L	
Density	kg/m^3
Heat capacity at constant pressure	$\mathrm{J}/(\mathrm{kg} \cdot \mathrm{K})$
Thermal conductivity	$\mathrm{W}/(\mathrm{m} \cdot \mathrm{K})$

Table 5.2: Material Descriptions

5.6 Laminar Flow

5.6.1 Governing Equations

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F} \tag{5.1}$$

where ρ is the density of air, $\mathbf{u}$ is the velocity vector, p is the pressure, $\mathbf{I}$ is the identity matrix, $\mathbf{K}$ is the viscous stress tensor, and $\mathbf{F}$ is the volume force vector.

$$\nabla \cdot (\rho\mathbf{u}) = 0 \tag{5.2}$$

$$\mathbf{K} = \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \tag{5.3}$$

where μ is the dynamic viscosity of air.

5.6.2 Initial Values

1. Velocity field

$$\mathbf{u} = \mathbf{0} \tag{5.4}$$

2. Pressure

$$p = 0 \tag{5.5}$$

5.6.3 Boundary Conditions

1. Wall (No slip)
$$\mathbf{u} = \mathbf{0} \tag{5.6}$$

2. Inlet (Velocity)
$$\mathbf{u} = -U_0\mathbf{n} \tag{5.7}$$
where U_0 is the initial velocity (i.e. normal inflow velocity) and $\mathbf{n}$ is the unit normal vector.

3. Outlet (Pressure)
$$[-p\mathbf{I} + \mathbf{K}]\,\mathbf{n} = -\hat{p_0}\mathbf{n} \tag{5.8}$$
$$\hat{p_0} \leq p_0, \nabla\mathbf{G}\cdot\mathbf{n} = 0 \tag{5.9}$$
where $\hat{p_0}$ is the estimated standard condition pressure, $p_0 = 0$ is the standard condition pressure (i.e. suppress backflow), $\mathbf{G}$ is the reciprocal wall distance.

4. Symmetry
$$\mathbf{u}\cdot\mathbf{n} = 0 \tag{5.10}$$
$$\mathbf{K}_n - (\mathbf{K}_n\cdot\mathbf{n})\mathbf{n} = 0, \mathbf{K}_n = \mathbf{K}\mathbf{n} \tag{5.11}$$

5.7 Heat Transfer

5.7.1 Governing Equations - Solid

$$\rho C_p\mathbf{u}\cdot\nabla T + \nabla\cdot\mathbf{q} = Q + Q_{ted} \tag{5.12}$$

where C_p is the specific heat capacity of air, T is the temperature of air, $\mathbf{q}$ is the heat flux vector, Q is the heat source, and Q_{ted} is the thermoelastic damping heat source.

$$\mathbf{q} = -k\nabla T \tag{5.13}$$

where k is the thermal conductivity.

$$Q = (1.23 - Operating\ Voltage) \times \frac{Fuel\ Cell\ Stack\ Current}{Cell\ Area} \tag{5.14}$$

5.7.2 Governing Equations - Fluid

$$\rho C_p\mathbf{u}\cdot\nabla T + \nabla\cdot\mathbf{q} = Q + Q_p + Q_{vd} \tag{5.15}$$

where Q_p is the point heat source.

$$\mathbf{q} = -k\nabla T \tag{5.16}$$

5.7.3 Governing Equations - Thin Layer

$$-\mathbf{n}_d \cdot \mathbf{q}_u = \frac{(T_u - T_d)}{R_s} + \frac{1}{2} d_s Q_s \tag{5.17}$$

where R_s is the thermal resistance, and d_s is the thin layer thickness.

$$-\mathbf{n}_u \cdot \mathbf{q}_u = \frac{(T_d - T_u)}{R_s} + \frac{1}{2} d_s Q_s \tag{5.18}$$

$$R_s = \frac{d_s}{k_s} \tag{5.19}$$

5.7.4 Initial Values

1. Temperature

$$T = T_{amb} \tag{5.20}$$

where T_{amb} is the initial ambient temperature.

5.7.5 Boundary Conditions

1. Insulation

$$-\mathbf{n} \cdot \mathbf{q} = 0 \tag{5.21}$$

2. Symmetry

$$-\mathbf{n} \cdot \mathbf{q} = 0 \tag{5.22}$$

3. Boundary Heat Source

$$-\mathbf{n} \cdot \mathbf{q} = Q_b \tag{5.23}$$

where Q_b is the boundary heat source.

4. Outflow

$$-\mathbf{n} \cdot \mathbf{q} = 0 \tag{5.24}$$

5. Inlet

$$T = T_{amb} \tag{5.25}$$

5.8 Mesh

5.9 Study

5.9.1 Difference between External and Internal Sweep

An internal sweep involves varying parameters directly within the simulation model itself. This type of sweep is integrated into the simulation process, where the solver automatically adjusts the parameters as part of its internal algorithm. Internal sweeps are typically used to explore the parameter space of the model in

a more automated and controlled manner, often leveraging the solver's built-in capabilities to iterate through different parameter values.

An external sweep, on the other hand, involves varying parameters outside of the simulation model. This is usually managed by an external script or control mechanism that systematically modifies the input parameters, runs the simulation for each set of parameters, and collects the results. External sweeps provide more flexibility and control over the parameter variations and can be useful for complex scenarios where the internal capabilities of the solver might be limited.

5.9.2 Parametric Sweep

A parametric sweep is a systematic method used in simulations and computational experiments to explore the effects of varying parameters within a defined range. By adjusting one or more input parameters incrementally, researchers can observe how changes influence the outcome, enabling a comprehensive analysis of the system's behavior. This technique is essential for optimizing designs, identifying critical factors, and understanding the sensitivity of the results to different variables. Ultimately, parametric sweeps provide valuable insights that drive informed decision-making and innovation.

Name	**Values**	**Unit**
Hcc	1 1.25 1.5 1.75 2	mm
Wcc	0.5 0.75 1 1.25 1.5	mm
Lcc	30 60 90	mm

Table 5.3: Parameter Sweep Values for All Combinations

5.9.3 Auxilary Sweep

An auxiliary sweep is a computational technique used to study the influence of secondary parameters or variables that are not directly part of the main parametric study. It involves varying these auxiliary parameters to investigate their impact on the primary simulation or experiment results. This approach helps in understanding the interactions and dependencies between primary and auxiliary parameters, providing a deeper insight into the system's overall behavior. Auxiliary sweeps are particularly useful in complex models where multiple factors may indirectly affect the outcomes, aiding in fine-tuning and enhancing the accuracy of simulations.

Name	Values	Unit
Uin	1 3.25 5.5 7.75 10	m/s
Q	1272 3132 5040	W/m^{-2}
Tamb	-20 0 20 40	°C

Table 5.4: Auxilary Sweep Values for All Combinations

5.10 Results

5.10.1 Accumulated Probe Table: Set 1

1. Hcc (1 - hc)
2. Wcc (2 - wc)
3. Lcc (3 - length)
4. Tamb (4 - Tamb)
5. Q (5 - Q)
6. Uin (6 - Uin)
7. Delp (15 - Pressure (Pa), Pressure Probe 3)

Figure 5.1: Pressure Probe 3 Location

8. Tsta (18 - Temperature (degC), Stack Temperature Probe 1)

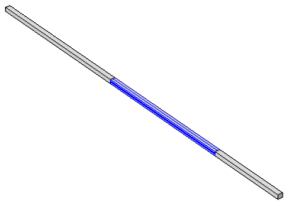

Figure 5.2: Stack Temperature Probe 1 Location

5.10.2 3D Plots

1. Pressure Drop

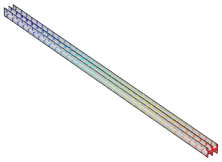

Figure 5.3: Pressure Drop 3D Plot

2. Temperature Stack

Figure 5.4: Temperature Stack 3D Plot

3. Velocity

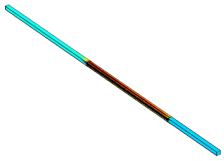

Figure 5.5: Velocity 3D Plot

5.11 Conclusion

5.12 Outlook

5.13 References