Artificial intelligence-assisted optimization and multiphase analysis of polygon PEM fuel cells

Ali Jabbary, Nader Pourmahmoud, Mir Ali Asghar Abdollahi, and Marc A. Rosen

ABSTRACT
This study introduces innovative, optimized hexagonal and pentagonal PEM fuel cell models. The inlet pressure and temperature serve as input parameters, while power consumption and output power are objective parameters. The results of Computational Fluid Dynamics (CFD) analysis are then trained with deep neural networks and modeled using polynomial regression. Target functions are derived using the Response Surface Method (RSM) and optimized with the NSGA-II genetic algorithm. Compared to the base model, our optimized pentagonal and hexagonal PEM fuel cells significantly boost the output current density by 21.8% and 39.9%, respectively. Additionally, power consumption is lower: the pentagonal model uses 0.198%, and the hexagonal model uses 6.21% of the production power on average. Our proposed designs enhance PEM fuel cell performance by significantly boosting power production while minimizing power consumption.

1. Introduction
Conventional fuel sources cannot fulfill our energy demands today, and their usage pollutes the environment significantly (Akorede, Hizam, and Pouresmaeil 2010). Renewable energy sources have gained reputations due to sustainability and fewer environmental side-effects (Owusu, Asumadu-Sarkodie, and Dubey 2016). Many researchers have studied and utilized Polymer Electrolyte Membrane Fuel Cells (PEMFCs) due to their ability to generate electrical energy through the electro-oxidation of fuel (Wang et al. 2011). PEM fuel cell is the most commonly utilized type of cell because of its quick starting time (Barbir 2006) and convenience in transportation (Peighambardoust, Rowshanzamir, and Amjadi 2010), and minor stationary energy requirements (Hamelin et al. 2001). Furthermore, the ever-increasing use of PEM fuel cells needs more research to make it more promising (Banham and Ye 2017).

The challenges that the PEM fuel cell faces are water and thermal management (Berg et al. 2004; Liu et al. 2020; Owejan et al. 2009; Oztürk and Yurtcan 2020; Rahimi-Esbo et al. 2017; Xu et al. 2020; Yuan, Ou, and Kim 2020; Zhang et al. 2020), performance optimization (Cai et al. 2020; Carcadea et al. 2020; Lan et al. 2020; Wang et al. 2020), design and modeling (Abdollahi et al. 2022; Cai et al. 2020; Mojica et al. 2020; Pan et al. 2020), and cell humidification (Cao et al. 2021; Liu et al. 2017; Shao et al. 2020; Subin and Jithesh 2018; Wilberforce et al. 2019; Zhao et al. 2018).

Ka’ki et al. (Ka’ki et al. 2021) developed a conductive nanocomposite membrane for high-temperature PEMFCs, demonstrating high proton conductivity at room temperature and after processing at 200°C. In a separate study, Taieb et al. (Taieb, Mukhopadhyay, and Al-Othman 2022) developed an adaptive estimation technique for PEMFC stack model parameters, enabling the prediction of fuel cell behavior with improved accuracy.

One of the critical topics that can be applied to achieve proper performance for the fuel cell is geometric design configuration (Wang 2015).

Bipolar plates (BP), gas channels, gas diffusion layers (GDL), catalyst layers (CL), and the polymer electrolyte membrane are the five essential components of a PEM fuel cell (Wang et al. 2011). The membrane electrode assembly (MEA) is placed between the current collectors. MEA comprises five parts, including a polymer electrolyte membrane, CL, and GDL at each end (Carcadea et al. 2020).

The cell’s geometric design and flow field are essential in fundamental parameters such as how the species are diffused, velocity, temperature and pressure distributions, liquid water content, and current density production (Berning, Lu, and Djilali 2002). Considerable study has been conducted on the cell structure to enhance its performance (Manso et al. 2012). Mass transfer, temperature diffusion, and electrochemical performance can be enhanced by initiating appropriate flow fields and decreasing pressure drop in the cell (Li and Sabir 2005; Wilberforce et al. 2019).

Dong et al. investigated the energy performance of a PEM fuel cell by using discontinuous S-shaped and crescent ribs into flow channels (Dong, Xie, and Ni 2021). Asadzade et al. simulated a new bipolar plate based on a lung-inspired flow field for PEM fuel cells to gain higher current densities (Asadzade and Shamloo 2017). Seyhan et al. used artificial neural networks to forecast the cell performance with wavy serpentine channels (Seyhan et al. 2017).

Shen et al. conducted a study where they introduced blockages in the flow channel of a Proton Exchange
Membrane Fuel Cell (PEMFC) to enhance mass transfer (Shen, Tu, and Chan 2019). Including these blockages improved the synergy angle between gas velocity and concentration gradient, resulting in an enhanced mass transfer coefficient and overall performance of the PEMFC. This innovative approach introduces a new dimension for optimizing flow field design.

In another research by Shen et al., they proposed a novel 3D flow field design for PEMFCs (Shen, Tu, and Chan 2020). This design aimed to improve mass transfer and eliminate liquid water through the sub-channel. It was observed that increasing the reactant inlet’s velocity proved advantageous for water removal. This study offers valuable insights into optimizing water transport and performance in PEMFCs.

Afshari et al. analyzed a zigzag flow channel design for cooling PEM fuel cell plates, and their design provided better temperature control in the cell (Afshari, Ziaei-Rad, and Dehkhordi 2017). Jabbary et al. performed a three-dimensional numerical study on a PEM fuel cell with a rhombus design. This study’s results indicate that this design significantly increases the power and current density (Jabbary et al. 2021). They conducted another study using a new cylindrical configuration on cell performance and water flooding (Samanipour, Ahmadi, and Jabbary 2020). This design reduces the amount of liquid water in MEA levels and prevents water flooding.

A useful way to increase the performance and output power is geometric or parametric optimization (Wang et al. 2017). Optimizing the fuel cell’s main parameters before the final operation is one of the most effective ways to reduce production and maintenance costs (Fletcher, Thring, and Watkinson 2016). Researchers used numerous methods for mathematical optimization in the fuel cell field. Bio-inspired methods like particle swarm (Sarma and Ganguly 2020) whale (El-Fergany, Hasanien, and Agwa 2019), genetic algorithm (Cai et al. 2020), Gray Wolf (Vatankhah Barenji, Ghadiri Nejad, and Asghari 2018), seagull (Lei, Song, and Rodriguez 2020), and fish swarm (Bai, Wang, and Wang 2017) methods are among these.

Cao et al. experimentally analyzed PEM fuel cells using a new, improved seagull optimization algorithm (Cao et al. 2019). In addition, Miao et al. introduced a new optimization method called the Hybrid Gray Wolf Optimizer to obtain the optimal parameters of the PEM fuel cell (Miao et al. 2020). Song et al. (Song et al. 2004) examined one- and two-parameter optimization analysis of the catalyst layer of the PEM fuel cell to maximize the current density of the catalyst layer with a given electrode potential.

The advantages of using the genetic algorithm are (Dehghanian and Mansour 2009; Sivanandam and Deepa 2008):

- Implementation of this theory is simple.
- It searches the population points, not a single point.
- It employs payout data rather than derivatives.
- It provides multi-target optimization.
- It does not utilize deterministic rules but employs probabilistic transitional rules.

Artificial intelligence (AI) can broadly be integrated as a fascinating modern technology with most research areas to solve challenges. As a result, this methodology has proved to have a high potential for advanced improvement in technological growth (Dwivedi et al. 2019). AI assists in the enhancement of performance and the development of new enterprise models (Wamba-Taguimde et al. 2020). In addition, embedded AI solutions can optimize manufacturing processes and extend machines and services with intelligent functions (Tao et al. 2018). As a result, artificial intelligence (AI) will be a critical component in the future competitiveness of mechanical engineering products and processes.

In one study, Su et al. developed an adaptive boosting charging strategy incorporating a capacity estimation method based on operation parameters (Su et al. 2022). This strategy, used for state estimation and adaptive adjustment during the charging/discharging cycling process, demonstrated a capacity loss limit of 4.44% and a significant decrease in average charging time.

In a separate study, Su et al. proposed a novel capacity prediction method for estimating lithium-ion batteries’ state of health (SOH) (Su et al. 2022). Based on the battery equivalent circuit model (ECM), deep learning, and transfer learning, this method showed ideal prediction performance when established using virtual data and the generative adversarial network (GAN)-based transfer learning method.

Dhimish et al. (Dhimish and Zhao 2023) developed a highly accurate ANN-based model for fault detection in PEM fuel cells, achieving a remarkable fault detection rate of over 93% for different types of faults. This work represents a significant advancement in fuel cell technology, enhancing reliability and lifespan.

Rezk et al. (Rezk et al. 2022) investigated the optimal parameter estimation strategy for PEM fuel cells in DC microgrids. Their study demonstrated the effectiveness of a Gradient-based optimizer in identifying the best parameters for different PEM fuel cells, highlighting the importance of accurate design and modeling for improving performance and reducing costs in PEMFCs.

Wilberforce et al. (Wilberforce et al. 2022) investigated the optimization of operating conditions to boost the output power of PEM fuel cells. By employing the particle swarm optimization (PSO) algorithm, they identified the best parameters, resulting in a significant increase in power output. The study concluded that the combination of fuzzy modeling and PSO achieved a power improvement of 5.26% and 9.38% compared to other methodologies and measured data, respectively.

Mei et al. (Mei et al. 2022) conducted research on optimizing operating and structural parameters of PEM fuel cells to improve power output. Through multi-objective optimization, they aimed to maximize power and efficiency while minimizing environmental impacts and cost. The study concluded that metal foam can enhance cooling efficiency and heat transfer in the fuel cell, suggesting its favorable use compared to nanofluid.

This study presents new pentagonal and hexagonal fuel cell designs. In multiphase analysis, optimization techniques based on artificial intelligence have been used to investigate the effects of critical parameters on current density and output/consumed powers. Furthermore, multiple analyses given the average cell’s pressure, temperature, velocity, and water content were performed to determine the performance of these models. This study aims to achieve maximum output power while maintaining minimum consumed power.

This study presents a novel approach to enhance the performance of Proton Exchange Membrane (PEM) fuel cells by
introducing pentagonal and hexagonal models to overcome the limitations of the current cubic model. The optimization process employs artificial intelligence techniques such as neural networks and genetic algorithms. The optimized pentagonal and hexagonal models significantly increase output current density, 21.8%, and 39.9%, respectively. Additionally, a comprehensive multiphase analysis considers various factors. These advancements have implications for improving efficiency and reliability in the industry. Figure 1 presents a diagram illustrating the research motivation underlying our investigation.

2. Methodology

2.1. Physical model

The fuel cell model based on CFD techniques numerically investigated physical and electrochemical phenomena. The base design of the fuel cell (Cubic) and the polygon models used in this research are shown in Figure 2, which shows the cell’s main components.

The sizes and geometric specifications are displayed in this figure and are described in Table 1.

2.2. Model assumptions

A comprehensive fuel cell is a highly complex device that includes fluid dynamics, mass transport phenomena, and electrochemical processes. The following simplification assumptions have been made to analyze a problem involving a three-dimensional model (Wang 2004):

- Channel flows are assumed to be laminar, incompressible, and steady;
- PEMFC operates in non-isothermal, multiphase, and steady-state situations;
- GDL and CL are isotropic and homogenous;
- The MEA (membrane electrode assembly) is homogenous porous media with uniform porosity;
- The membrane is entirely humidified, ensuring consistent ionic conductivity.

Compared to the base design, the basis for the different inlet/outlet areas and channel lengths in the pentagonal and hexagonal models is rooted in optimizing the fuel cell performance. The new designs aim to enhance the performance of PEM fuel cells by overcoming the limitations in generating current density and electrical power inherent in the cubic model. The different inlet/outlet areas and channel lengths in the pentagonal and hexagonal models result from this optimization process, which uses artificial intelligence techniques such as neural networks and genetic algorithms.

In addition, the justification for these differences is to keep the wet area of the Membrane Electrode Assembly (MEA) constant and equivalent for all of the models. This is crucial because the MEA is the heart of the fuel cell where the electrochemical reactions occur. By keeping the wet area of the MEA constant, we ensure that the active area, where the fuel and oxidant are converted into electricity, remains the same across all models. This allows for a fair comparison of the different models’ performance, as any performance changes can be

![Figure 1. Research motivation.](image)

![Figure 2. PEM fuel cell models (sizes are in mm).](image)
attributed to the design of the model rather than differences in the active area.

For our research, we analyzed the PEM fuel cell models using numerical analysis techniques instead of experimental methods. Experimental analyses of PEMFCs make several simplifying assumptions. These include:

- Steady-state operation.
- Isothermal operation.
- Ideal gas behavior.
- Homogeneous catalyst.
- Negligible mass transport losses.
- Negligible ohmic losses.
- Negligible crossover.

While numerical modeling allows complex fuel cell phenomena analysis, experimental validation remains essential. Experimental studies provide real-world data to test the accuracy of PEMFC models and assumptions. Addressing the idealizations in numerical analyses through targeted experimentation can help identify the most critical non-ideal phenomena and improve future fuel cell designs.

### 2.3. Governing equations

Reactive flow, species transfer, reactive consumption, water production, temperature and pressure diffusion are only a few factors that must be studied to evaluate cell performance. Different variables are studied using a three-dimensional steady-state model.

#### 2.3.1. Continuity equation

The conservation of mass equation (continuity) in all regions is (Atyabi and Afshari 2019):

$$ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 $$

(1)

Electrodes are manufactured by carbon cloth or carbon fiber (Zhou et al. 2016). Therefore, they are recognized as a porous medium where distributed reactant gases (species). Concerning the porosity of MEA (\(\varepsilon\)), the continuity equation is given by:

$$ \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = S_m $$

(2)

\(u\), \(v\), and \(w\) are velocity in the \(x\), \(y\), and \(z\) axes, individually, \(\rho\) is the density of reactant gases. \(S_m\) is the mass sink/source term, which is considered zero since no reaction occurs in the flow channels and GDLs. However, because of the reactivity of reactant species, the sink/source term is not zero in the catalyst layer and can be evaluated by (Toghyani et al. 2018):

$$ S_{H_2} = -\frac{M_{H_2}}{2F}R_a $$

(3)

$$ S_{O_2} = -\frac{M_{O_2}}{4F}R_c $$

(4)

$$ S_{H_2O} = +\frac{M_{H_2O}}{2F}R_c $$

(5)

\(F\) is the Faraday constant \((96,485\,\text{C}/\text{mol})\), and \(M\) is the species’ molecular weight \((\text{kg}/\text{mol})\) and \(R\) can be calculated by Butler–Volmer Equations (18 and 19).

#### 2.3.2. Momentum equations

The momentum conservation equations:

$$ \nabla \cdot (\rho \vec{u}) = -\nabla P + \nabla (\mu \nabla \vec{u}) + S_{p,i} $$

(6)

\(S_{p,i}\) is the sink/source term for porous media in the \(x\), \(y\), and \(z\) axes. As the pressure decreases in porous media, Darcy’s law has been estimated in the model. The source term is (Das, Mukherjee, and Muralidhar 2018):

$$ S_{p,i} = -\left( \sum_{i=1}^{3} \frac{1}{\beta_i} \mu u_i \right) $$

(7)

\(\beta\) is the permeability of the media.

#### 2.3.3. Energy conservation

The energy conservation equation:

$$ \nabla \cdot (\rho C_p \vec{u} T) = \nabla \cdot (k_{eff} \nabla T) + S_h $$

(8)

where \(k_{eff}\) denotes effective thermal conductivity, \(C_p\) denotes specific heat at constant pressure, and \(S_h\) is the additional volumetric source term in the energy equation. \(k_{eff}\) is calculated by:

$$ k_{eff} = \epsilon k_f + (1 - \epsilon)k_s $$

(9)

And \(S_h\) is evaluated by:

$$ S_h = h_{react} - R_{an,cat} \eta_{an,cat} + \tilde{I}^2 R_{ohm} + h_L $$

(10)
\( h_{\text{react}} \) represents the net change in enthalpy caused by electrochemical reactions. The ohmic term is estimated because there is no heat production operator in bipolar plates. As a result, the energy equation is reduced to:

\[
\nabla \cdot (k \nabla T) = -R_{\text{ohm}} I^2
\]

(11)

\( k \) is the conductivity of the bipolar plates.

### 2.3.4. Mass transfer (species transport equations)

The reactant gases are hydrogen and air, which can be assumed to behave as ideal gases. The following are the equations for species transport:

\[
\nabla \cdot \left( \varepsilon_i \nabla C_i \right) = \nabla \cdot \left( D_i^{\text{eff}} \nabla C_i \right) + S_i
\]

(12)

\( C_i \) is the species' molar concentration, \( S_i \) is the extra volumetric source term of species such as \( H_2, O_2 \), and \( H_2O \) for CLs zones and are calculated by:

\[
S_{H_2} = - \frac{R_a}{2F}
\]

(13)

\[
S_{O_2} = - \frac{R_c}{4F}
\]

(14)

\[
S_{H_2O} = \frac{R_c}{2F}
\]

(15)

In addition, the gas diffusivity coefficient \( D_i^{\text{eff}} \), which is determined by operation conditions, is provided by (Ghasabehi, Jabbary, and Shams 2022):

\[
D_i^{\text{eff}} = \epsilon^{1.5} (1 - s)^{2.5} (D_i^0 \frac{P_0}{P}) (\frac{T}{T_0})^{1.5}
\]

(16)

\( r_i \) is the saturation exponent of pore blockage, \( D_i^0 \) is the reference mass diffusivity of the \( i \)-th species under standard conditions, and \( s \) is water saturation (the volume percentage of liquid water) and is derived as follows:

\[
s = \frac{V_{\text{liquid}}}{V_{\text{total}}}
\]

(17)

\( V \) is the volume.

### 2.3.5. Butler–Volmer equation

The Butler–Volmer equation can define the volumetric transfer currents as follows (Ghasabehi, Jabbary, and Shams 2022; Ghasabehi, Shams, and Kanani 2021):

\[
R_a = (\zeta_{\text{el}} \beta_{\text{el}})^{\varepsilon_a} \left( \frac{C_{H_2}}{C_{H_2}^0} \right)^{\gamma_a} \left( e^{\frac{nF \Delta \phi_a}{RT_{\text{ref}}}} - e^{-\frac{nF \Delta \phi_a}{RT_{\text{ref}}}} \right)
\]

(18)

\[
R_c = (\zeta_{\text{el}} \beta_{\text{el}})^{\varepsilon_c} \left( \frac{C_{O_2}}{C_{O_2}^0} \right)^{\gamma_c} \left( -e^{\frac{nF \Delta \phi_c}{RT_{\text{ref}}}} + e^{\frac{nF \Delta \phi_c}{RT_{\text{ref}}}} \right)
\]

(19)

The values \( \beta_{\text{el}}, \zeta, \) and \( \alpha \) represent the reference exchange current density, specific active surface area, and transfer coefficient. In addition, \( \varepsilon, \varepsilon_{\text{ref}} \), and \( \gamma \) represent the concentration of reactant flow, the reference value, and the concentration dependency, respectively.

### 2.3.6. Charge conservation equations

Electrochemical processes take place at the catalyst layers in PEM fuel cells. Surface activation overpotential is the main factor behind these responses (Sivertsen and Djilali 2005). Therefore, the potential difference between the solid and the membrane is referred to as the activation overpotential (Das, Li, and Liu 2008). As a consequence, two charge equations are required. One equation for electron transport via conductive solid phase and another for proton transport across the membrane:

\[
\nabla \cdot (\sigma_{\text{sol}} \nabla \phi_{\text{sol}}) + R_{\text{sol}} = 0
\]

(20)

\[
\nabla \cdot (\sigma_{\text{mem}} \nabla \phi_{\text{mem}}) + R_{\text{mem}} = 0
\]

(21)

Current density \( (A/m^2) \) is used to describe volume sink terminology. Only in the catalytic layers are these expressions set. For the solid phase, they are calculated by:

Anode side:

\[
R_{\text{sol}} = -R_a \quad (<0)
\]

(22)

Cathode side:

\[
R_{\text{sol}} = +R_c \quad (>0)
\]

(23)

For the membrane phase, they can be evaluated by the following equations:

Anode side:

\[
R_{\text{mem}} = +R_a \quad (>0)
\]

(24)

Cathode side:

\[
R_{\text{mem}} = -R_c \quad (<0)
\]

(25)

The following equation is used to determine the average current density:

\[
i_{\text{ave}} = \frac{1}{A} \int_{V_a} R_a dV = \frac{1}{A} \int_{V_c} R_c dV
\]

(26)

### 2.3.7. Water transport via membrane

Water produced by the cathodic process in PEM fuel cells diffuses to the anode side. It will transport across the membrane via electro-osmosis force and back diffusion (Das, Li, and Liu 2010). \( \lambda \) is determined as the number of water molecules divided by the number of charged HSO_3 sites. Springer et al. (Springer, Zawodzinski, and Gottesfeld 1991) developed a formula for estimating it:

\[
\lambda = \begin{cases} 
0.043 + 17.81a - 39.85a^2 + 36a^3 & a < 1 \\
14 + 1.4(a - 1) & a > 1
\end{cases}
\]

(27)

\( a \) denotes the water activity.

### 2.3.8. Consumption and production powers

The consumption and production powers are two important parameters affecting the performance of the PEM fuel cell. The specified values are obtained and examined in section 3. The
following equations can be used to determine these parameters (Jabbary et al. 2021):

- Production power:
  \[ P_{pro} = I \cdot V \cdot A_{eff} \] (28)

- Consumption power:
  \[ P_{cons} = \Delta P \cdot A_{in} \cdot u_{in} \] (29)

Here, \( A_{eff} \) is the effective area of the membrane, and \( A_{in} \) is the inlet area of the channel.

### 2.4. Cost function

In the context of this research, the cost function serves as a mathematical tool that quantifies the performance of the fuel cell models. The goal is to optimize this cost function to achieve the best performance. Specifically, the optimization process aims to maximize the fuel cell models’ output power (Production Power) while minimizing the power they consume (Power Consumption).

\[ \text{Cost} = -P_{pro} + \lambda \cdot P_{cons} \] (30)

Where:
- \( P_{pro} \) represents the production power of the cell.
- \( P_{cons} \) represents the consumption power of the cell.
- \( \lambda \) is the weighting factor determining the importance or weight given to the consumption power in the cost calculation.

The value of \( \lambda \) depends on the relative importance of the two objectives. If the Production Power is more important than the Power Consumption, \( \lambda \) should be less than 1. The exact value of \( \lambda \) should be determined based on the specific requirements and constraints of the project. For example, if the Production Power is twice as important as the Power Consumption, \( \lambda \) might be set to 0.5. This means that for every unit increase in Power Consumption, the Production Power needs to increase by two units to maintain the same cost.

### 2.5. Simulation conditions

Table 2 demonstrates the initial operating conditions utilized for numerical simulation providing the same initial operating conditions to all models.

The boundary conditions of the models are given in Table 3, and the specifications of the MEA layers are shown in Table 4 according to Hashemi’s study (Hashemi, Rowshanzamir, and Rezakazemi 2012).

### 2.6. Numerical procedure

Figure 3 displays the presented CFD algorithm of PEM fuel cell simulation. ANSYS® Fluent 2021 software was used in CFD analysis to solve the governing equations through computational domain using the finite volume method.

The double-precision and second-order upwind methods were applied to discretize the terms. In addition, the multigrid \( F \)-Cycle type (Mulder 1989) and the BCGSTAB method (BiConjugate Gradient Stabilized Method) with 50 max course cycles were employed to stabilize the solutions and avoid divergence due to the complex nature of the governing equations.

Stopping criteria are requirements that must be met for the algorithm to be stopped. Since an iterative approach

| Table 2. Operating conditions of the fuel cell models. |
|------------------------------------------------------|
| Parameter                                      | Unit   | Value  |
| Operating pressure                             | Pa      | 101325 |
| Operating temperature                          | K       | 353.15 |
| Anode relative humidity                        | %       | 100    |
| Cathode relative humidity                      | %       | 100    |
| Anode stoichiometry                            | –       | 1.2    |
| Cathode stoichiometry                          | –       | 2      |

| Table 3. Boundary conditions of the fuel cell models. |
|------------------------------------------------------|
| Parameter                                      | Unit   | Cubical | Pentagonal | Hexagonal |
| Anode mass flow rate                            | kg/s   | 1.3e-07 | 1.3e-07 | 1.3e-07 |
| Cathode mass flow rate                          | kg/s   | 1.4e-06 | 1.4e-06 | 1.4e-06 |
| mass fraction at anode inlet                    | –      | 0.113   | 0.113   | 0.113   |
| mass fraction at cathode inlet                  | –      | 0.886   | 0.886   | 0.886   |
| mass fraction at cathode inlet                  | –      | 0.151   | 0.150   | 0.151   |
| mass fraction at cathode inlet                  | –      | 0.353   | 0.353   | 0.353   |
| Inlet pressure                                  | atm    | 1       | 1       | 1       |
| Relative inlet humidity                         | %      | 100     | 100     | 100     |
| Inlet temperature at anode/cathode              | K      | 353.15  | 353.15  | 353.15  |

| Table 4. Membrane Electrode Assembly (MEA) properties. |
|------------------------------------------------------|
| Parameter                                      | Symbol | Unit   | Value  |
| GDL porosity                                    | \( \varepsilon_{GDL} \) | – | 0.5   |
| CL porosity                                     | \( \varepsilon_{CL} \) | – | 0.5   |
| Membrane porosity                               | \( \varepsilon_{mem} \) | – | 0.6   |
| Electrical conductivity of electrode            | \( \sigma_{ele} \) | S/m | 100   |
| Proton conductivity of membrane                 | \( \sigma_{mem} \) | S/m | 17.1  |
| Thermal conductivity of electrode               | \( k_{th} \) | W/mK | 1.3   |
| Anode apparent charge transfer coefficient      | \( q_{an} \) | – | 0.5   |
| Cathode apparent charge transfer coefficient    | \( q_{cat} \) | – | 1.0   |
| Anode exchange current density                  | \( R_{an}^{ex} \) | A/m² | 30    |
| Cathode exchange current density                | \( R_{cat}^{ex} \) | A/m² | 0.004 |
computes successive approximations to a nonlinear system’s solution, a test is required to decide when to terminate the iteration. Stopping criteria would evaluate the distance between the latest iteration and the correct answer. These distances are called residuals. The lower the value of residuals, the closer the numerical analysis results to the existing solutions with fewer errors. When the residuals reach the desired value, the iteration is over, and the final results will be obtained.

2.7. Assumptions and sources of error

Our study made several key assumptions:

- The reactant gases (hydrogen and air) were assumed to behave as ideal gases.
- The electrodes were assumed to be a porous medium where distributed reactant gases (species).
- The conservation of mass equation (continuity) in all regions was applied.
- The double-precision and second-order upwind methods were applied to discretize the terms.
- The multigrid F-Cycle type and the BCGSTAB method (Biconjugate Gradient Stabilized Method) with 50 max course cycles were employed to stabilize the solutions and avoid divergence due to the complex nature of the governing equations.

Despite these assumptions, we recognize that there are potential sources of error in our study:

1. Errors in the numerical solution of the governing equations due to discretization and iterative solution methods.
2. Errors due to the idealization of certain phenomena, such as the behavior of the reactant gases and the porosity of the electrodes.
3. Errors in estimating specific parameters, such as the effective thermal conductivity and the additional volumetric source term in the energy equation.
4. Errors due to the assumptions made in the multi-objective optimization process, such as the selection of the objective functions and the choice of the optimization algorithm.

2.8. Artificial intelligence-assisted optimization

Mathematical optimization is an effective method for resolving complex problems by utilizing the most efficient resources and data. Optimization is determining the values of decision variables to achieve a problem’s goal. One of the most important applications of artificial intelligence is lowering the computing costs of optimization. An optimization model comprises appropriate objectives, variables, and constraints. The most reliable solution is choice variables that maximize or minimize the objective function while remaining within the solution range. The objectives of this study are the produced and consumed powers. Feed-forward deep neural networks were used to model the data. Response Surface Method (RSM) was applied for function approximation to extract objective functions and use them in the optimization algorithm.

2.8.1. Machine learning model

Figure 4 shows the deep neural network for modeling the objectives and variables. A sequential model for the neural network was created using Tensorflow (Abadi et al. 2016). The mentioned neural network has two input neurons (inlet temperature and inlet pressure) and one output neuron (once for produced power and once for consumed power) with two hidden layers, each with ten neurons. Relu activation function
was applied for the hidden layers. After modeling the data, two-dimensional polynomial regression was used to obtain the objective functions.

### 2.8.2. Genetic algorithm

The genetic algorithm is a heuristic optimization strategy replicating natural evolution by changing a population of individual solutions (Fogel 1994). Chromosomes represent design points \( x \). The method selects parents randomly from the existing population and uses them to produce the next generation. Since good parents produce good children, the population gradually approaches an ideal solution over successive generations. The algorithm eliminates the bad points from the generation. GA can achieve the optimal global solution without clinging to a locally optimal solution. Because GA is a probabilistic method, different runs may yield different results. As a result, many iterations are required to validate the best solution.

The genetic algorithm consists of five stages:

- **Initial population**: The procedure starts with a group of data identified as a population. Each case is a potential solution to the addressed problem; Genes are a set of characteristics (variables) that describe a person. Chromosomes comprise a string of genes (solution).

- **Fitness function**: The fitness function defines an individual’s fitness level. It assigns each case a fitness score, determining the likelihood of an individual being chosen for regeneration.

- **Selection**: This stage aims to choose the fittest individuals and pass on their genes to the next generation. Two sets of individuals are selected depending on overall fitness levels. Individuals with high fitness scores are more likely to be determined for regeneration.

- **Crossover**: Crossover is the most critical stage. A crossover point is a randomly selected point within the genes for each couple of parents to be matched.

- **Mutation**: The mutation stage is to conserve population variety and prevent early convergence.

When the population convergence is achieved, the algorithm is terminated, and the solutions are obtained.

### 3. Results and discussion

This section will present the results, analyze the fundamental parameters of the models, and compare them. The grid independence test and model validation are explained in our previous work (Jabbar et al. 2021).

#### 3.1. Optimization

The desired parameters of the problem are mathematically optimized. The input parameters of this research are the inlet pressure and temperature of the cell, and the output parameters are power consumption and production power. Our goal is to maximize output power while maintaining/minimizing power consumption. To perform this, the inlet pressure was changed from 1 atm to 5 atm and the inlet temperature from 50°C to 90°C at the same time. Step. At each stage, consumption and production power were calculated. **Figure 5** Shows the changes of these powers with different pressures and temperatures in three-dimensional space.

Production power in both models has the highest values at all temperatures and a pressure of 1 atmosphere – the higher the inlet pressure, the lower the production power. **Figure 6** shows the two-dimensional contours of these results. The power consumption in the two models, at all pressures and a temperature of 90°C, has its maximum values. By decreasing the temperature, the power consumption of the fuel cell can be reduced.

The data were modeled using the neural network shown in **Figure 4** to perform multi-objective optimization. Then, with multi-parameter polynomial regression, the mathematical relations of the problem objectives were obtained. The relationships for power production are as follows:

![Feed-forward neural network](image-url)
Upon establishing the objective functions for the problem, denoted by $P_{pro}$ and $P_{cons}$, we employed the robust NSGA-II multi-objective genetic algorithm for optimization. Opting for two hundred generations, a population size of 200, and a random seed of 1, we have meticulously shaped the optimization process. Figure 7 elucidates the optimal range between the two objective functions, demonstrating the fruits of our optimization efforts.

As per the insights derived from this figure, a clear pattern emerges in both models: an increase in production power invariably leads to an uptick in the fuel cell's consumption power. Such findings warrant a careful evaluation to identify
optimal values for the problem’s input parameters. Interestingly, the power consumed by the device in both models significantly trails behind the production power, accounting for merely 0.198% and 6.21% of the production power in the Pentagonal and Hexagonal models, respectively.

In light of this, should the maximum production power be harnessed in both models, the power consumption would be a mere fraction of the production power—0.25% in the Pentagonal model and 8.29% in the Hexagonal model. Consequentially, even if the input parameters are manipulated to yield the maximum output power, the power consumption remains substantially lower, reinforcing the efficiency of our models.

We have meticulously identified the optimized parameters for both Pentagonal and Hexagonal models in this study. To ensure exemplary performance, we have strategically set the inlet pressure and temperature for the Pentagonal model at 1 atm and 77.645 °C, respectively. Similarly, these parameters for the Hexagonal model are established at 1 atm and 90 °C. With these values carefully calibrated, we forge ahead with our analysis, anticipating promising results that testify to our rigorous approach.

### 3.2. Polarization curves and current density

Figure 8 shows the polarization curves of the presented models. The presented models produced more current and power density than the Cubic model. The performance of the optimized models in this field is more than the standard models due to optimized parameters. To compare these values accurately, Table 5 and Figure 9 indicate the percentage increase in the current density of the proposed models.

First, standard models perform better than base models. The Pentagonal and Hexagonal models have an average current density of 19.096% and 15.179% higher than the base model. Second, the current densities generated by the optimized models are even higher than the standard models, shown in Figure 9. The optimized pentagonal and hexagonal
models have an average current density of 21.819% and 39.931% higher than the base model.

Two main reasons for these enhancements are optimal parameters and the new cell design. The performance of the presented models at near-open voltage is relatively similar to the cubic model. However, at low voltages, their performance has significantly enhanced.

The superior performance of the models presented in this study, particularly their ability to generate higher current and power density compared to the cubic model, can be attributed primarily to two key factors: optimal parameters and innovative cell design. The optimization process, which used artificial intelligence techniques, enabled us to meticulously fine-tune the fuel cell models’ parameters to achieve maximum efficiency.

On the other hand, introducing pentagonal and hexagonal designs offers a more efficient arrangement for the fuel cell components, leading to performance improvements. These new designs facilitate better distribution of both fuel and oxidant, resulting in more effective electrochemical reactions and, consequently, higher current and power densities.

It is worth noting that the performance of the presented models is relatively similar to that of the cubic model when
operating near-open voltage. However, under low voltage conditions, their performance exhibits significant enhancements, highlighting the effectiveness of the new designs and optimized parameters in such scenarios.

### 3.3. Effects of relative humidity

Figure 10 displays the effect of Relative Humidity (RH) on the performance of the standard presented fuel cell models. Humidity is among the main factors influencing fuel cell performance. Decreasing RH causes a reduction in the membrane’s proton transfer conductivity in both cases. Overall, decreasing RH may decrease electrode kinetics, including electrode reaction, mass diffusion rates, and membrane proton conductivity, leading to a severe decrease in cell efficiency. According to this result, 100% humidity is reported to achieve adequate performance for both models.

Humidity plays a significant role in the performance of Proton Exchange Membrane (PEM) fuel cells. Humidity notably influences the performance of Proton Exchange Membrane (PEM) fuel cells, as demonstrated by Mittermeier et al. (Mittermeier et al. 2018). Their study revealed that reducing relative humidity (RH) from 100% to 25% at 80°C resulted in a substantial decrease in carbon oxidation reaction (COR) during start-up/shut-down events, directly affecting fuel cell performance. Additionally, Nishimura et al. (Nishimura et al. 2022) found that the impact of RH on temperature distribution at the reaction surface was more pronounced at higher initial temperatures, further affecting fuel cell performance. These findings confirm the observations presented in Figure 10 of our paper, confirming the significant influence of humidity on PEM fuel cell performance.

### 3.4. Liquid water content

The amount of liquid water in the MEA influences the proton conductivity and the activation overpotential. If MEA is not sufficiently hydrated, proton conduction drops and cell...
resistance increases. On the other hand, surplus water can cause problems in fuel cells, including water flooding. Figure 11 shows the volumetric average of water content in the standard models’ layers. Since this content is minimal in the anode part, the cathode sections’ water content was displayed. The water content at humidities below 100% is minimal in the fuel cell layers. This reduction in water content may cause the membrane to dry out and ultimately reduce the efficiency of the fuel cell.

The amounts of water in both models are close to each other. At 0.355 V and 0.375 V, the cathode layers of both the hexagonal and pentagonal models contain the highest water content.

3.5. Potential assembly into a stack

In the context of our research, we have proposed two novel designs for Proton Exchange Membrane (PEM) fuel cells: the pentagonal and hexagonal models. While our analysis primarily focused on the performance of individual cells, it is essential to consider how these cells could be assembled into a stack, as this is the typical configuration in practical applications of fuel cells.

In the potential stacked structures of the presented models, each cell, consisting of an anode, a cathode, and a PEM sandwiched between them, would be held together by a bipolar plate. This plate would be designed to match the cells’ shape and facilitate efficient gas distribution. The individual cells would then be stacked on top of each other, with insulating...
materials between each cell to prevent electrical shorting. The stack would be compressed to ensure good contact between the components and to minimize electrical resistance.

Figure 12(a, b) illustrate the potential stacked structures for the pentagonal and hexagonal models. As shown in these figures, the unique shapes of our proposed designs could offer advantages in terms of packing efficiency and gas distribution in the stack. However, it is essential to note that these figures represent conceptual illustrations of the potential stacked structures, and further research is needed to validate these designs and analyze their performance in a stacked configuration.

By considering the potential assembly of our proposed designs into a stack, we hope to provide a more comprehensive understanding of their potential applications and pave the way for future research in this area.

4. Conclusion

This paper presented two new designs for PEM fuel cells with pentagonal and hexagonal shapes. They were optimized after obtaining an increase in the performance of these models compared to the cubic model in generating current density and electrical power. The data were trained using neural networks and regression techniques. The Response Surface Method (RSM) was applied to derive the mathematical function corresponding to the problem objectives: production and consumption power. Using a multi-objective genetic optimization algorithm (NSGA-II), the targets were simultaneously optimized for problem inputs, including operating temperature and pressure. The optimized results were compared to the results of standard models once the optimum settings for these models were determined. In addition, the effects of changes in the relative humidity of the cell inlet in the models were analyzed, and the liquid water content was investigated.

The optimal designs outperform the base model (Cubic Model) and are more effective than the standard models. The average increase in output current density of the optimal models compared to the base model (Cubic) is 21.8% and 39.9% in the pentagonal and hexagonal models. Compared to optimized and standard cases, the mentioned percentage is 2.7% and 24.7% in the pentagonal and hexagonal models. The effect of relative humidity (RH) on the channel inputs of standard models was investigated. 100% humidity is the optimal setting for achieving the highest possible current density in the models. Reducing the relative humidity of the inlet causes the MEA to dehydrate, reducing the current density and ultimately reducing the cell efficiency. The cathode section layers measured the average volumetric volume of liquid water content. For standard pentagonal and hexagonal models, the corresponding voltages for the highest liquid water contents are 0.379 V and 0.355 V.

The results of this study are essential for the fuel cell industry. Novel pentagonal and hexagonal fuel cell designs have been fine-tuned using artificial intelligence methods, substantially increasing output current density. The optimized pentagonal and hexagonal models exhibited improvements of 21.8% and 39.9%, respectively, when compared to the standard model. This boost in performance has the potential to enhance energy production efficiency, resulting in reduced operational expenses and potentially making fuel cell technology more accessible and viable for a broader range of applications. Incorporating artificial intelligence into the optimization process presents exciting possibilities for advancing and refining fuel cell technology. The discoveries made through this research hold immense potential to revolutionize the fuel cell industry by propelling technological advancements and contributing to the overarching objective of sustainable and efficient energy production.

These are some of the potential implementations of the results in the industry:

- Energy Efficiency: Optimized fuel cell models enhance energy efficiency in industries, reducing costs through increased current density.
- Sustainable Energy Solutions: Enhanced fuel cell models support creating sustainable energy solutions, including electric vehicles and stationary power generation.
- Space and Aeronautics: These fuel cells’ compact and efficient design makes them ideal for weight-sensitive space and aeronautics applications.
- Portable Power Devices: Enhanced fuel cell designs extend battery life and optimize power usage in portable devices like laptops and mobile phones.
- Artificial Intelligence in Energy Systems: AI-driven fuel cell optimization strategies enhance efficiency across various energy systems.

4.1. Highlights

This section highlights the introduction of novel pentagonal and hexagonal Proton Exchange Membrane (PEM) fuel cell models that aim to overcome the limitations of the current cubic model. It emphasizes using AI-assisted optimization techniques and multiphase analysis to enhance current density and power output. The optimized models demonstrate substantial performance improvements with potential implications for the industry.

- **Novel Design:** Introduced new pentagonal and hexagonal Proton Exchange Membrane (PEM) fuel cell models, aiming to overcome the limitations of the current cubic model in generating current density and electrical power.
- **AI-Assisted Optimization:** Utilized artificial intelligence techniques, including deep neural networks and genetic algorithms, for optimizing the parameters of the new fuel cell models.
- **Multiphase Analysis:** Conducted a multiphase analysis to investigate the effects of critical parameters on current density and output/consumed powers.
- **Performance Enhancement:** The optimized pentagonal and hexagonal models increased the output current density by 21.8% and 39.9%, respectively, compared to the base model.
- **Impact on Industry:** The research results can significantly improve the efficiency and reliability of PEM fuel cells, having substantial implications for the industry.
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