Modelling and Optimization of a Microbial Fuel Cell

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Annex A

THESIS ACCEPTANCE CERTIFICATE

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DEDICATION

I would like to dedicate my thesis to my parents and my siblings, who have always been supporting me and motivating me to study. I would like to express my gratitude to my parents who have always believed in me and encouraged me to work hard in the completion of this thesis. All the hard work, time, and understanding I have received from them have been very inspiring and I am grateful for it.

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ABSTRACT

Microbial Fuel Cells (MFCs) are an innovative technology that stands at the intersection of renewable energy production and wastewater treatment. MFCs provide a sustainable solution for the production of energy by utilizing the metabolic processes of microbes to transform organic substrates into electrical energy. MFCs model must be optimized to improve their performance. Due to some problems such as low power density, substrate constraints, and inefficiencies in electron transmission, MFC can’t achieve their potential.

In this study we have adopted a comprehensive mathematical model for MFCs, incorporating critical factors like electron transmission, microbial activity and substrate consumption. This thesis investigates the application of advanced optimization techniques to improve MFC performance metrics, particularly focusing on current output and overall efficiency. To replicate MFC operations, a thorough mathematical model is adopted, taking into account important variables including anodic and cathodic reactions, microbial activity, and substrate concentration.

In order to optimize MFC parameters, the study uses Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimization (GWO), and Gradient-Based Optimization (GBO). Through comparative evaluations of numerical simulations, the effectiveness of various methods is assessed. The outcomes reveal substantial improvements in current output, with GWO exhibiting remarkable efficiency in systems with complicated dynamics and GA and PSO obtaining greater enhancements in the earlier phases. Despite being less computationally demanding, GBO offers a reliable starting point for parameter optimization.

The study's conclusion highlights the necessity of interdisciplinary approaches to fully realize the potential of this sustainable technology and offers insights into how optimization techniques will be integrated into MFC design in the future.

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Chapter 1: Introduction

1.1 Background:

As the global demand of energy surges, to address the major concern like environmental concerns, resource depletion, and the need for sustainable development the shift from conservative fossil fuels to the renewable energy resources have become important. Microbial Fuel Cells, are one of the many cutting-edge technologies which provide a unique solution by merging wastewater treatment with the production of renewable energy. MFCs provides dual benefits of waste remediation and power generation by using the metabolic activity of microbes to convert organic matter in wastewater into electrical energy. [1]

Microbial Fuel Cells (MFCs) have gained significant attention as an eco-friendly solution for power generation and wastewater treatment during the past 20 years [1]. MFCs generate energy by first breaking down organic compounds in substrates utilising the metabolic processes of microorganisms, which releases electrons as a byproduct that may be captured and used to generate power [2]. Because MFCs can cleanse wastewater and generate electricity, they are at the intersection of biotechnology, environmental engineering, and electrochemistry [3]. Researchers are attempting to improve the practical feasibility of MFCs through various options like novel materials, reactor designs, and optimization. Optimization improvements have increased in the previous few years, particularly since 2020 [4]. The use of optimization, from traditional gradient-based approaches to more modern metaheuristics techniques like Genetic Algorithms (GA), Particle Swarm Optimization (PSO), and Grey Wolf Optimizer (GWO), to optimize power output and to improve substrate utilization, and to reduce operating costs, MFCs are one of the most promising developments [5].

Although MFCs have a lot of potential but there are still major complications to overcome, Scaling up to real-world applications also requires addressing various problems like electrode material enhancement, membrane and reactor design complexity, and the variety of organic matter in actual wastewater, even though laboratory scale MFCs have shown that they are feasible to convert the chemical energy stored in organic substrates into electrical energy [6]. Since MFCs often work with complicated water metrics such as suspended solids, variable pH, fluctuating chemical Oxygen Demand (COD), and the presence of inhibitory compounds, water optimization is one of the main crucial area among these issues [7]. Pre-treatment water parameter optimization can greatly increase MFC performance, lower costs, and improve the sustainability of these systems.

In order to increase MFC efficiency, this study explores the fundamentals of MFCs, the main issues that hinder it performance, and the various optimization techniques that have regularly being used, ranging from population-based metaheuristics techniques like GA, PSO, and GWO to classical approaches such as gradient-based methods..

1.2 Problem Statement

MFCs are still very much under-utilized in real-world and it's applications are limited despite their potential overcome energy crisis in major world countries. Its applications are being limited because of it's inefficiencies that affects their operational performance and hence their scalability.

The main problems consist of:

- Their limited ability to move electrons from the cathode to anode, which lowers their output current.
- Microorganism inability to perform activity and it's inability to fully deplete the substrate during prolonged operation.
- Suboptimal parameter configurations, such as electrode characteristics and microbial concentration are also a major concern

In order to overcome these obstacles and systematically enhance MFC performance, sophisticated mathematical modelling and optimization approaches must be integrated.

1.3 Objectives:

This study and thesis objective is to investigate various optimization techniques to enhance the performance of the Microbial Fuel Cell:

- To develop a mathematical model of Microbial Fuel Cell that takes into account the important factors like electrode reactions, substrate utilization, and microbial activity in order to depict the activities of the Microbial Fuel Cell.
- The utilization of the cutting-edge optimization techniques to improve performance metrics, Optimization techniques like Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimization (GWO), and Gradient-Based Optimization (GBO).
- Comparing various optimization methods in order to determine which one is best for increasing system efficiency and current output.

1.4 Scope of Study

The following are included in the study's scope:

- The development of a mathematical model for the operation simulation of MFC.
- The use of gradient-based optimization methods to adjust parameters.
- Comparative evaluation of algorithms using data from simulations.
- Suggestions for incorporating optimal parameters into MFC design for real-world use.

Chapter 2: Literature Review

2.1 Overview of Microbial Fuel Cell (MFC)

Microbial Fuel Cells are one of the cutting-edge technology that can provide solution to two major global issues at once: waste-water treatment and the production of renewable energy. The microbe's capability to break down organic materials and release electrons in the process and it forms the basis of MFC technology. A sustainable energy source is produced by using these electrons, electrical energy is produced.

Potter initially proposed the idea of harnessing biological processes to generate energy in 1911 after proving that bacteria could produce current [8]. But MFC research didn't really take off until the early 2000s, thanks to developments in environmental engineering, materials science, and microbiology. The foundation for contemporary MFC design was established by studies by Logan et al. [9] and Rabaey et al. [10], which improved performance by refining reactor designs and electrode materials.

- Key Developments in MFC Design

Research into MFC design has focused on improving power density, enhancing microbial electron transfer efficiency, and reducing costs. Significant advancements include: The main area of study is electrode material. The development of high-surface-area electrodes, like those made of carbon, to promote electron transport and microbial colonisation [11]. Another area of key development is membrane technology. Proton exchange membranes (PEMs) and other materials are introduced in membrane technology to lower internal resistance and enhance ionic conductivity [12]. One area of development is related to microbial selection.

To optimize current generation, electrochemically active bacteria like Shewanella and Geobacter species are isolated and genetically modified [13]. Reactor Configuration is also been developed recently. To enable scalable applications, move from basic two-chamber configurations to sophisticated single-chamber and stacked systems [14].

2.1.1 Types of MFC Configurations

Several MFC configurations exist, each tailored to specific substrates, operational conditions, or desired outcomes. Common types include: Main Chamber MFC, Dual-Chamber MFC, Air Cathode MFC and Stacked MFC. Each one is explained individually

- **Single-Chamber MFC**: The cathode is either submerged in the same chamber as the anode or exposed to air in a single compartment. Although this design is simpler, oxygen diffusion may limit power output [14].
- **Dual-Chamber MFC**: A membrane divides the anode and cathode chambers. By keeping cathodic processes isolated from the surroundings of the anode chamber, this design enhances them; nevertheless, it may also result in an increase in internal resistance [8].
- **Air-Cathode MFC**: By eliminating the need for a catholyte and external aeration, a specialised single-chamber design that exposes the cathode to air on one side can save operating expenses [15]
- **Stacked MFC**: To attain greater voltages or currents, many MFC units are stacked in parallel or series. Although stacking facilitates scaling, it can be difficult to regulate each unit's performance [16].

2.1.2 Applications of MFCs

MFCs have been researched for:

- Waste water streams from industry, agriculture, and municipalities are being treated. [17].
- The production of electricity, hydrogen (in microbial electrolysis cells), and other products with added value commonly known as Bioenergy Generation**.**
- The ability to detect pollutants or biochemical oxygen demand (BOD) in real time [18].
- The process of recovering metals and nutrients (such as phosphate and nitrogen) from waste streams is known as Resource Recovery [19].
- The focus on integrated systems, which combine MFCs with other treatment methods like anaerobic digestion or built wetlands, has increased since 2020 since they provide complementary advantages for resource recovery and energy production [20].

2.2 Fundamentals of Microbial Fuel Cells (MFCs)

2.2.1 What are Microbial Fuel Cells (MFCs)

Microbial Fuel Cells (MFCs) are an innovative bioelectrochemical technology that aims to solve two major worldwide issues: wastewater treatment and sustainable energy production. MFCs generate electricity from organic substrates by utilising the inherent metabolic processes of electrochemically active microorganisms. MFCs are positioned as an innovative approach for integrated energy and environmental applications because of their dual functionality.

2.2.2 Description of the Microbial Fuel Cell Schematic

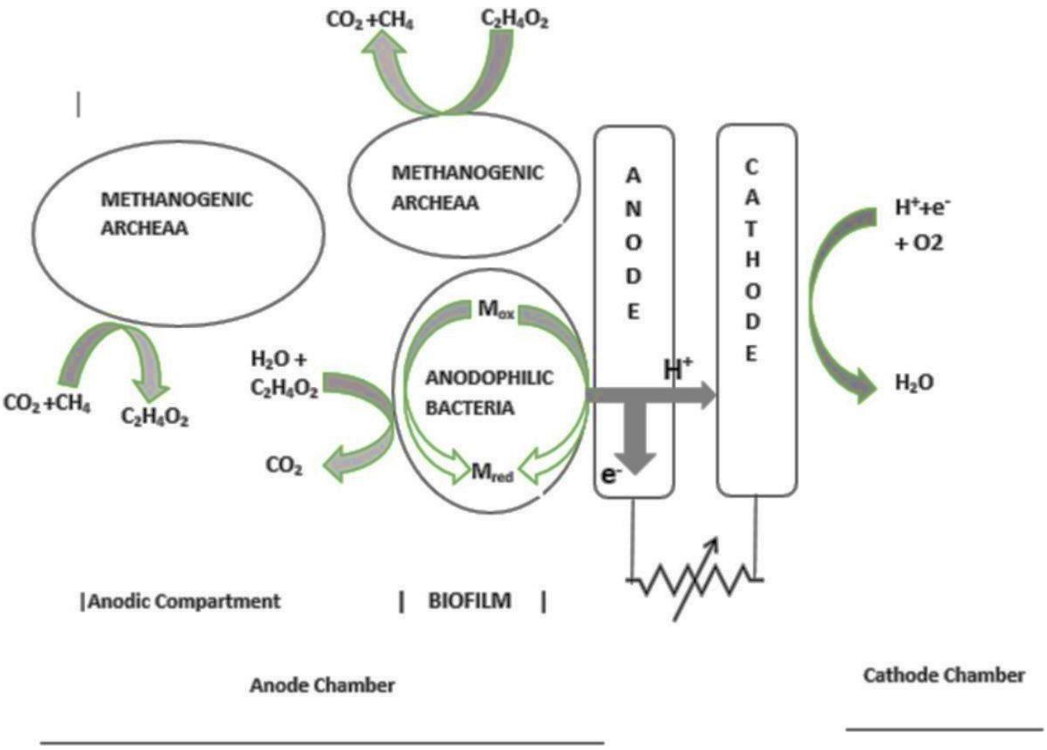

Figure 1 - Schematic Diagram of MFC

The figure highlights the function of microbial communities, electron transport, and electrochemical reactions taking place in the anode and cathode chambers as it depicts the operation of a microbial fuel cell (MFC).

- **Anodic compartment:**

Anodophilic bacteria are essential for oxidising organic substrates in the anode chamber, including acetate ($C_2H_4O_2$) or other carbon sources, generating carbon dioxide (CO_2), protons (H^+), and electrons (e^-).

Microbial electron mediators switch between their oxidised (M_{ox}) and reduced (M_{red}) states to transfer electrons to the anode during the oxidation processes, which are a redox cycle.

- **Biofilm Formation:**

At anode surface, a biofilm made up of microbes to promotes effective electron transfer and substrate breakdown. Electron recovery from organic materials is improved by this biofilm.

- **Methanogenic Archaea:**

In the anode chamber, methanogenic archaea cohabit and transform substrates such as hydrogen and CO_2 into methane (CH_4), a competitive process that lowers the amount of electrons available for power generation. To maximise the MFC's performance, this interaction must be balanced.

- **Electron Transfer to the Cathode:**

An electrical current is created when the electrons produced in the anode chamber move through an external circuit. This flow is in charge of supplying electricity to loads or external devices.

- **Proton Exchange:**

To keep the system's charge balanced, protons (H^+) diffuse to the cathode chamber via a proton exchange membrane (PEM).

- **Cathodic Compartment:**

Water (H_2O) is created at the cathode when protons and electrons mix with oxygen (O_2). The electrochemical process cannot be completed without this oxygen reduction reaction.

- **Energy Output:**

The potential difference between the two electrodes determines the voltage, whilst the flow of electrons from the anode to the cathode produces a detectable current. These all work together to influence the MFC's power output

2.2.3 Principle of Operation

The unique abilities of electroactive microorganisms to transform chemical energy that exists in organic substrates into electrical energy is the foundation of a Microbial Fuel Cell's (MFC) functioning. The oxidation of organic materials, electron transport via a circuit, and reduction processes at the cathode are all components of this bioelectrochemical process. As explained below, the smooth integration of biological, chemical, and electrochemical processes is essential to the system's effectiveness.

- **Anode Chamber:**

The anode chamber is a space deprived of oxygen that is host to electroactive microbes. Through metabolic activities, these microorganisms decompose organic substrates, such as glucose, acetate, or wastewater constituents. While this deterioration is occurring

- **Electron and Proton Release:**

Microbes oxidise organic substrates, which causes protons and electrons to be released.

$$\mathbf{C_6H_{12}O_6+6H_2O \rightarrow 6CO_2+24H^{+}+24e^{-}} \quad \mathbf{(1)}$$

- **Electron transport:**

Microbial electrochemical pathways either directly or indirectly transport electrons to the anode through conductive electron shuttles (mediators) .

As the anode itself accepts electrons in this anaerobic environment, metabolic functions continue unhindered.

- **Proton Exchange Membrane (PEM)**

The proton exchange membrane (PEM) allows the protons produced in the anode chamber to move to the cathode chamber. For the system to remain stable, this selective membrane is essential because:

Keeping oxygen from leaking into the anode chamber and only permitting protons to flow through. Maintaining constant electron flow across the external circuit by balancing the ionic charges between the two chambers.The MFC's total performance is directly impacted by the PEM's efficiency. Although their cost and durability continue to be issues, materials like Nafion are frequently utilised for this purpose.

- **Cathode Chamber**

Reduction processes take place in the oxygen-rich cathode chamber. Here, protons from the PEM and oxygen from the surroundings interact with the electrons that have passed through the external circuit to create water:

$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \quad (2)$$

Since it "closes the loop," completing the electrical circuit and permitting continued electron flow, this reaction is crucial. High conductivity and corrosion resistance are requirements for the cathode material. Furthermore, the effectiveness of the reduction reactions is directly impacted by the availability of oxygen or another terminal electron acceptor.

- **External Circuit: The Pathway for Electrons**

Through an external circuit, the electrons released at the anode are guided to the cathode. An electrical current produced by this electron movement can be used for useful purposes. A number of variables affect the current's magnitude, including:

- the anode's microbial activity.
- he external circuit's resistance.
- the effectiveness of pathways for electron transport.

- **Energy Output and Application**

Microbial metabolic activity is the direct cause of the current produced by MFCs. Typically, the energy output is stated as follows:

$$P = V.I$$

where V is the external circuit's voltage, P is its power output, and I is its current. Because typical MFCs have modest power densities (mW/m2), optimization is essential for real-world uses

Chapter 3: Mathematical Modelling

3.1 Mathematical Model

A microbial fuel cell (MFC) can be mathematically modelled to illustrate the complex relationship of chemical, biological, and electrochemical processes. The model enables us to forecast important system variables including substrate consumption, microbial growth, current generation, mediator concentration, and system resistances across time by modelling these phenomena through a system of differential equations. A thorough examination of the mathematical formulas governing the MFC and how each affects the system's overall performance can be found below. The mathematical model is being adapted from Pinto et al., 'A two-population bio- electrochemical model of a microbial fuel cell,' 2010

3.1.1 Substrate Consumption and Biomass Growth Equations

Consumption of substrate is one of a microbial fuel cell's primary roles. The organic substrate (such acetic acid) is consumed by anodophilic bacteria, which help produce energy, and methanogenic archaea, which produce methane as a byproduct. These processes are captured by the following substrate consumption equation:

$$\frac{dS}{dt} = -\left(q_a \cdot x_a\right) - \left(q_m \cdot x_m\right) + D \cdot (S_o - S) \quad \textbf{(3)}$$

Where:

- S = substrate concentration at any given time
- q_a = reaction rate of anodophilic bacteria
- q_m = reaction rate of methanogenic archaea
- x_a = concentration of anodophilic biomass
- x_m = concentration of methanogenic biomass
- D = dilution rate
- S_o = initial substrate concentration

The equation 3 has several impacts on the overall working of the system. The first one being the substrate degradation. The equation illustrates how microbial consumption causes a gradual drop in substrate concentration. Methanogens use the organic substrate to produce methane, whereas anodophilic bacteria oxidise it to release protons and electrons. The second one is competing biomass. The consumption of substrate by both anodophilic (xa) and methanogenic (xm) biomasses creates a competitive dynamic that impacts the overall performance of MFCs. While methanogenic activity converts energy into methane, decreasing electrical efficiency, more anodophilic activity encourages the production of electricity. One of the impact it has is on dilution rate. To simulate feed or washout conditions, the term $D \cdot (So - S)$ describes how substrate flows into or out of the system.

Similarly equation 3 has several contribution to the system. One of the main is it show how much substrate is depleted. As anodophilic bacteria and methanogenic archaea consume the organic substrate, the concentration of the substrate decreases, as the equation illustrates. Current generation and the rate of microbial development are directly impacted by this depletion. The other contribution it shows the competition between the microbes. Methanogenic archaea (x_m) and anodophilic bacteria (x_a) compete for the same substrate, while methanogenic activity directs energy towards the generation of methane while anodophilic activity contributes to electrical output.

3.1.2 Current Generation Equation

In a microbial fuel cell, the flow of electrons from the anodic chamber through the external circuit generates current. This process is captured in the current equation:

$$\boldsymbol{I_{MFC} = \frac{E_{ocv}}{R_{ext} + R_{int}} \times \left(\frac{M_{red}}{\epsilon + M_{red}}\right) \quad (4)}$$

Where:

- I_{MFC} = current generated by the MFC
- E_{ocv} = open circuit voltage
- R_{ext} = external resistance
- R_{int} = internal resistance
- M_{red} = reduced mediator concentration
- ϵ\epsilonϵ = small constant to prevent division by zero

The equation 4 has some impact on overall system. The main thing this equation shows the current generated by MFC. The current generated by the MFC is directly defined by this equation. While higher resistances R_{ext} and R_{int} decrease the current, higher levels of E_{ocv} and M_{red} enhance it. The second thing equation 2 shows the concentration of mediate material. M_{red} is a symbol for the reduced mediator that transfers electrons between the electrode and bacteria. The current generated increases with the concentration of $M_{red.}$ The influence of resistance can also be seen through this equation. Internal resistance R_{int} is dependent on microbial activity and the conductivity of the MFC components, whereas external resistance R_{ext} is usually determined by the external load. The efficiency of current generation is decreased by a higher R_{int}. Similarly equation 4 has some contribution in the overall system. This equation directly tell us the electrical current generation. The open circuit voltage, resistances, and mediator concentration all affect the current generated by the MFC, which is measured by this equation. Better current generation is facilitated by reduced resistances and higher mediator concentrations. Secondly, it shows us interaction between voltage and resistance. The equation shows that system resistances (Rext, Rint) and open circuit voltage (Eocv) are directly related, with higher resistance reducing current.

3.1.3 Oxidized Mediator Concentration Equation

The concentration of the oxidized mediator (Mox) changes dynamically as a result of microbial activity and the current produced by the MFC. This is described by the following equation:

$$\frac{dM_{ox}}{dt}=(- Y \times q_a \times x_a)+(\gamma \times(\frac{I_{MFC}}{m \cdot F}) \times (\frac{1}{V \cdot x_a})) \quad (5)$$

Where:

- M_{ox} = concentration of the oxidized mediator
- Y = yield coefficient of the reaction
- q_a = anodophilic reaction rate
- x_a = concentration of anodophilic biomass
- I_{MFC} = current generated by the MFC
- m = number of electrons transferred
- F= Faraday’s constant
- γ\gamma = step rate
- V= volume of the microbial fuel cell.

The equation 5 has some impact on overall system. The main being it showed the balance between the mediator. The equilibrium between the rate at which anodophilic bacteria oxidise the mediator and the rate at which the current generated reduces it is modelled by this equation. The concentration of the oxidised mediator decreases with increasing Y·qa·xa, which impacts electron transport. The second thing it impact is electron transport. The current generation and mediator concentration are connected by the term ($\frac{IMFC}{}$). More oxidized mediator is decreased as IMFC rises, generating a feedback loop that can either limit or accelerate the present generation. One of the impact of equation 5 is on biomass concentration. The mediator concentration is also influenced by the amount of anodophilic biomass, or xa. Generally speaking, higher biomass results in higher mediator turnover, which affects the electrical output of the entire system. Similarly equation 3 has some contribution to the overall system. This equation contribute how mediator dynamics effects current. The above equation simulates how microbial activity and current generation affect the concentration of oxidised mediators over time. A dynamic balance in mediator concentration results from the reduction of more oxidised mediator as current generation rises. This equation also contribute towards efficiency of electrons transfer. A significant factor in electron transfer efficiency is mediator concentration; higher mediator turnover results in more effective electron transport and increased current generation.

3.1.4 Internal Resistance Equation

Internal resistance (R_{int}) is influenced by several factors, including the concentration of anodophilic biomass. The relationship between R_{int} and x_a is described by:

$$\mathbf{R_{int} = R_{min} + (R_{\mathit{max}} - R_{min}) \cdot e^{-Ks \cdot xa}} \quad \textbf{(6)}$$

Where:

- R_{int} = internal resistance
- R_{min} = minimum internal resistance
- R_{max} = maximum internal resistance
- K_s = rate constant related to biomass concentration
- x_a = concentration of anodophilic biomass

The equation 6 has some impact on overall system. It show the dependency of resistance over biomass concentration. R_{int} declines exponentially when the anodophilic biomass (x_a) concentration rises. Better conductivity and fewer internal energy losses result from this. The equation has some impact on current. A lower internal resistance leads to a higher production of current since Rint is present in the denominator of the current equation. Therefore, electrical performance is increased is directly related with the increase of biomass growth. The equation (4) also work as the limiting factor. For current generation, high R_{int} values serve as a limiting factor because of low biomass concentration. The equation (4) aids in estimate how the overall performance and resistivity of the system is being affected by the variations in microbial activity affect Equation 4 contributes in some way to the system as a whole. It demonstrates the connection between biomass concentration and resistance. As the anodophilic biomass (xa) concentration increases, internal resistance decreases exponentially. This boosts electron transport efficiency and generates more current. It demonstrates the clear connection between resistance and biomass. Microbial growth and internal resistance are directly correlated, as evidenced by the fact that increased microbial activity reduces resistance and improves system performance.

. 3.1.5 Open Circuit Voltage Equation

The open circuit voltage (Eocv) is an important parameter that governs the potential difference between the anode and cathode. It is modeled as an exponential function of the anodophilic biomass concentration:

$$\mathbf{E_{ocv} = E_{min} + (E_{max} - E_{min}) \cdot e^{-\frac{1}{Ks \cdot xa}}} \quad \mathbf{(7)}$$

Where:

- E_{ocv} = open circuit voltage
- E_{min}= minimum open circuit voltage
- E_{max}= maximum open circuit voltage
- K_s= rate constant related to biomass concentration
- x_a= concentration of anodophilic biomass

The equation 7 has some impact on overall system. The biomass concentration has some impact on voltage. The open circuit voltage approaches E_{max} as the anodophilic biomass (x_a) concentration rises. This increases the MFC's capacity to produce electricity. This equation also influence the current generation. Larger open circuit voltages result in larger current generation since Eocv is present in the current equation's numerator. The above equation connects the MFC's total electrical output to microbial growth. In short the system efficiency is directly been influenced by this. The MFC's operating limits are determined by the difference between E_{min} and E_{max}. System performance is maximised when the voltage is pushed closer to E_{max} by effective microbial growth.

The equation 7 has some contribution to the overall system. This equation show us the voltage control. The open circuit voltage gets closer to E_{max} as anodophilic biomass increases, which raises the potential difference between the anode and cathode. The current generation is better as a result. It shows relation relationship between biomass contribution and voltage generation. The relationship between biomass and voltage highlights how microbial growth directly impacts the voltage potential; larger biomass concentrations lead to higher voltages and improved system performance.

3.1.6 Overall System Dynamics

The microbial fuel cell's overall behaviour is described by the equations for substrate consumption, biomass growth, current production, mediator dynamics, internal resistance, and open circuit voltage. Changes in one of these interrelated equations have an impact on the others: The first being the biomass growth. Higher anodophilic bacterial concentrations result in higher current generation, less internal resistance, and enhanced electron transfer. The second being the substrate availability. Microbial activity slows down with decreasing substrate concentration over time, which lowers current generation and raises internal resistance. The third being mediator concentration. The ratio of reduced to oxidised mediators influences electron transfer rates, which in turn affects current generation and system performance as a whole. The fourth being resistance. Lower resistances allow for more effective energy conversion, and both internal and external resistances are essential in restricting current generation.

In conclusion, an MFC's mathematical model provides a thorough framework for comprehending the ways in which different chemical, biological, and electrochemical processes interact to convert organic substrates into electrical energy. In order to optimize and analyse MFC performance under various operating settings, each equation helps predict important system variables.

3.2. Mathematical Model Visualization:

OUTPUT GRAPHS:

The graphs shown below are the output visualizations of the mathematical model that we have adapted and being implemented in this work. This mathematical model has been coded using python language; due to its strong optimization and flexibility in creating customized scripts.

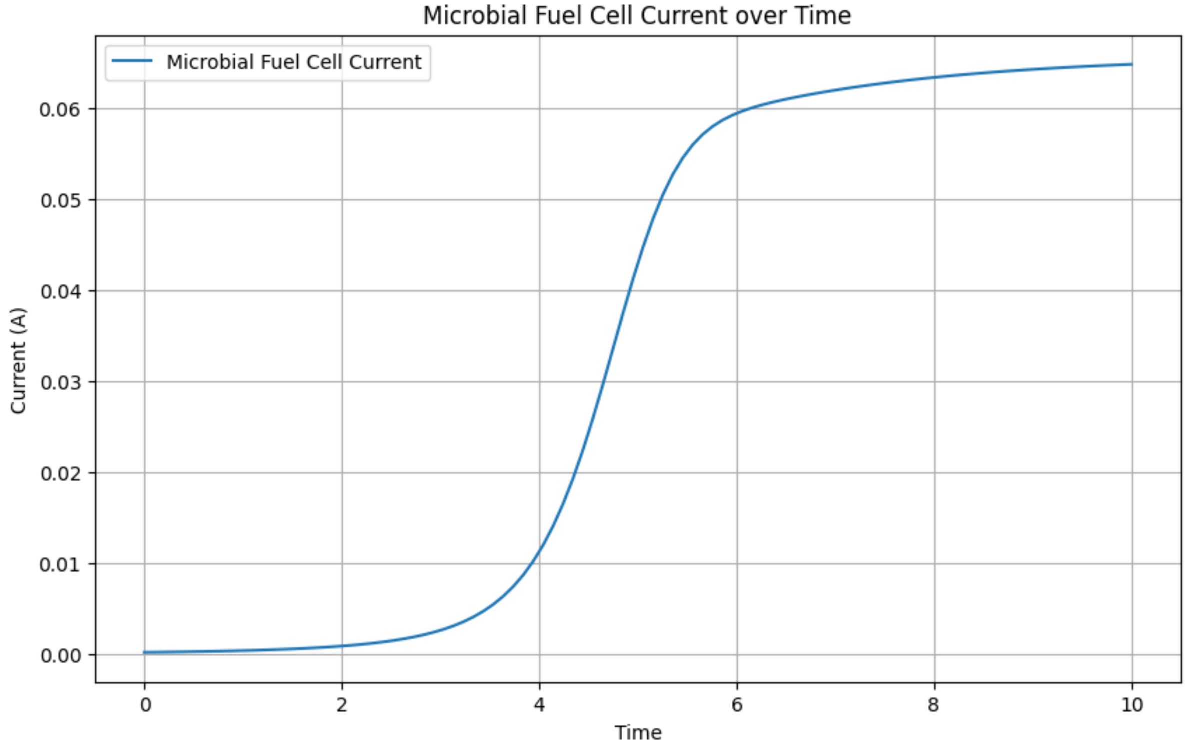

Figure 2 - Current graph before Optimization

- The Figure 2 shows the microbial fuel cell's current (IMFC) output with time. Since the electrochemical and microbiological processes are still in their infancy, the current is first very low, almost nothing.
- A rapid increase in current output occurs after a lag of roughly 4 seconds, indicating the start of effective microbial metabolism and substrate breakdown. This sharp rise marks the MFC's entry into the active phase of electron transfer and production.
- This plateau denotes the point at which substrate availability and microbial activity balance out, preventing additional current increases without optimization.
- Despite the system's steady-state behaviour, performance needs to be improved because the peak current is below ideal for the majority of energy applications.

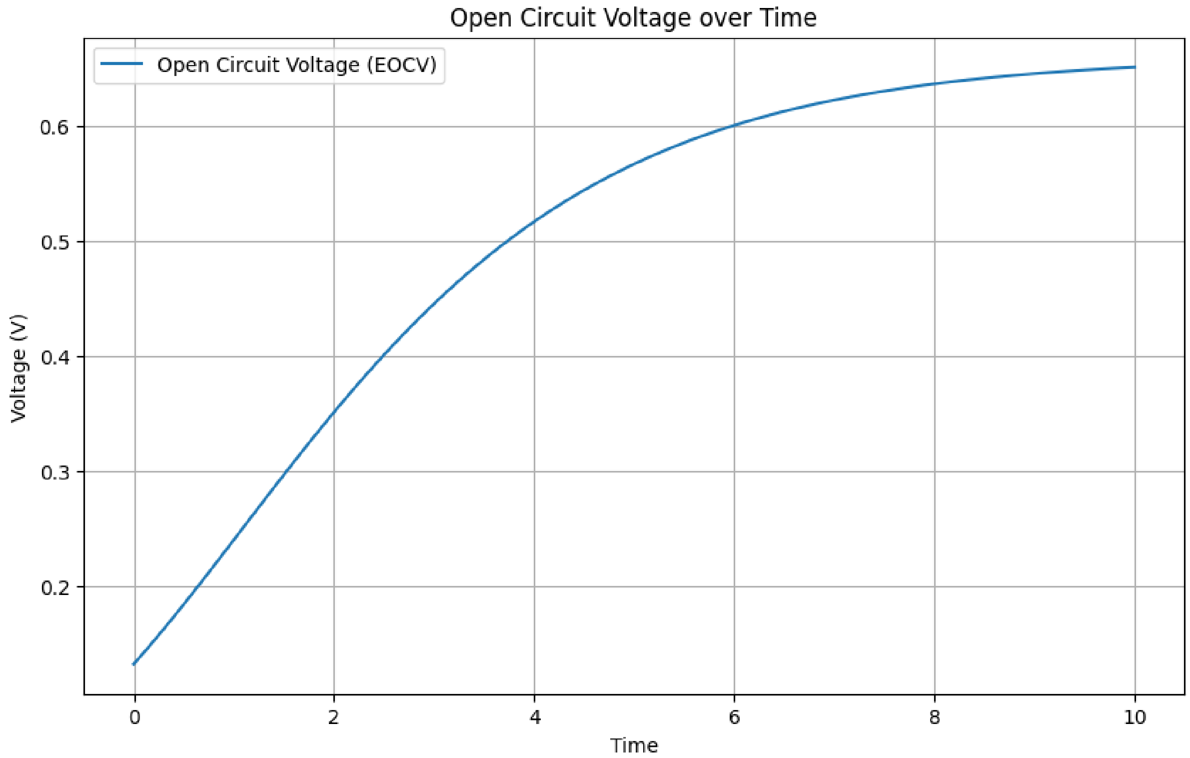

Figure 3 - Voltage graph before Optimization

- The Figure 3 shows how the open-circuit voltage (EOCV) changes over time. Since the cell has not yet reached steady state and the early electrochemical processes are slow, the voltage starts out low.
- The voltage gradually increases over time before stabilising at about 0.6 V. Based on the anode and cathode processes, this figure represents the thermodynamic limit of the MFC's energy conversion capacity.
- The efficiency of the system is limited by overpotentials, internal resistance, and electrode restrictions, even though the voltage level seems enough.

3.3 Importance of Current Enhancement Over Voltage Enhancement

3.3.1 Direct Impact on Power Output:

A microbial fuel cell's power output ($P = V \times I$) is exactly proportional to the product of voltage and current. Increasing the current is a more effective and realistic way to increase power output because MFC voltage is naturally constrained by thermodynamics.

Although the voltage in the unoptimized MFC is comparatively constant, the total power generation is severely constrained by the low current output. As a result, increasing the current becomes crucial to obtaining significant energy outputs.

3.3.2 Influence on Electrode Efficiency:

The efficiency of electron transfer from the anode to the cathode, which is influenced by the kinetics of the electron mediator, substrate availability, and microbial community activity, is linked to current generation. Current can be significantly increased by optimising these parameters.

However, intrinsic losses such concentration polarisation, ohmic resistance, and activation overpotentials at the electrodes limit voltage enhancement. Redesigning the cell structure is frequently necessary to address these losses, which is less practical than optimising parameters to increase current.

3.3.3 Scalability and Real-World Applications:

Higher current levels are needed to meet load needs in the majority of real-world energy applications, such as charging batteries or powering small devices. To make the MFC more useful, system optimizations might increase the current even at low voltages.

External electronic circuits, like as DC-DC converters, can be used to increase voltage, but the MFC's biological and electrochemical processes must be improved internally in order to increase current.

3.3.4 System Constraints and Optimization Focus:

The characteristics of the electrode material and the thermodynamics of chemical reactions have the biggest effects on the relatively constant voltage in an MFC. Consequently, without major structural alterations, increasing voltage is naturally constrained.

On the other hand, current is dynamic and closely related to operational elements including electrode surface area, substrate concentration, and microbial activity. Significant gains in current can be achieved by fine-tuning these parameters, which will raise the total power output. The pre-optimization performance patterns show the unoptimized microbial fuel cell's limitations in terms of both current and voltage outputs. Achieving realistic power production levels requires giving priority to current enhancement using optimization approaches as Genetic Algorithm (GA), Particle Swarm Optimization (PSO), Grey Wolf Optimization (GWO), and Gradient-Based Optimization (GBO). In addition to optimising power, current augmentation meets practical needs for scalable and effective energy systems, guaranteeing MFC technology's wider acceptance.

Chapter 4: Optimization

4.1 : Challenges in Microbial Fuel Cell

4.1.1 Power Density Limitation

MFCs frequently generate lower power densities than traditional fuel cells, despite much study [32]. Limited power outputs are caused by a number of factors, including internal resistance, electron transfer bottlenecks, and poor microbial activity. Optimising system components becomes crucial when researchers go towards real-world applications in order to close the gap between laboratory performance and real-world needs [33].

4.1.2 Internal Resistance and Energy Loss

Resistance of electrodes and electrolytes, charge transfer resistance at the electrode interface, and mass transfer limits are some of the causes of internal resistance in MFCs [34]. Cell voltage is lowered and total energy efficiency is decreased by high internal resistance.
Researchers can determine the ideal ratio of electrode spacing, membrane characteristics, and substrate flow rates to reduce these losses by using computer models and optimization techniques [35].

4.1.3 Scalability Issues

It is still difficult to scale MFCs from lab-scale (millilitres or litres) to larger pilot- or industrial-scale systems [36]. Issues including unequal substrate distribution, trouble sustaining anaerobic conditions, and a higher risk of biofilm detachment are brought about by larger systems. Scale-up issues may be resolved by combining strong optimization strategies with the application of sophisticated monitoring and control algorithms [37].

4.1.4 Complex Water Matrices in Real-World Wastewater

Complex matrices with differing quantities of heavy metals, organic and inorganic contaminants, and inhibitory substances (such as sulphides and ammonia) are present in actual wastewater streams [17]. Such intricacy may harm electrode materials or reduce microbial activity. These problems can be lessened by water optimization techniques, which range from pre-treatment to adaptive control of operating parameters. Computational and optimization tools are needed to determine the ideal operating parameters (pH, flow rate, and external resistance) under dynamic water matrix conditions [38].

4.2 Necessity of Optimization in Microbial Fuel Cells

The potential of Microbial Fuel Cells (MFCs) as a sustainable solution for wastewater treatment and energy generation is enormous. However, inefficiencies and restrictions including poor power density, inefficient substrate utilisation, and cost limits make it difficult to put them into practice. In order to overcome these obstacles and enhance MFC performance generally, optimization is essential.

4.2.1 Enhancing Power Output

Power density maximisation is one of the main objectives of MFC optimization. Internal resistance, electrode material characteristics, and microbial activity are some of the variables that affect an MFC's output. Suboptimal energy production could result from these characteristics operating below their potential if they are not optimized. It has been demonstrated that methods including adjusting microbial growth conditions, refining electrode design, and choosing the best substrates can greatly increase power output.

4.2.2 Improving Substrate Utilization

The concentration of substrates has a direct effect on MFC performance; efficient substrate use ensures that the most organic matter is transformed into electrical energy; optimization techniques assist in determining the optimal microbial communities and substrate concentration, minimising waste and increasing efficiency.

4.2.3 Addressing Material and Design Constraints

Performance is significantly impacted by the materials used for MFC components, such as electrodes and membranes. Conventional trial-and-error methods of choosing materials are costly and time-consuming. Optimization techniques, including computer simulations, make it possible to find affordable materials with improved performance attributes.

4.2.4 Reducing Operational Cost

By increasing system efficiency, optimization also seeks to lower operating expenses. MFCs can become more economically feasible by reducing energy losses, improving reactor designs, and strengthening material durability.

4.2.5 Utilizing Advanced Computational Techniques

Advanced computer techniques including Genetic Algorithms (GA), Particle Swarm Optimisation (PSO), Grey Wolf Optimisation (GWO), and Gradient-Based Optimisation (GBO) provide reliable solutions for improving MFC parameters. These techniques enable effective exploration of vast parameter spaces and the identification of optimal combinations for specific applications.

Future developments as well as existing MFC designs depend on optimisation. As novel microbial strains and materials are created, optimisation will be essential to incorporating these developments into useful systems. Furthermore, there is potential for real-time MFC operations optimisation through the application of AI and machine learning. Optimisation guarantees that this technology may be used successfully for environmentally friendly energy production and management by tackling the complex issues related to MFCs.

4.2.6 Optimization Objectives

In general, MFC research aims to optimize:

- The main objective of this optimization is to maximise power output.
- Making certain that organic matter breaks down more completely. Thus, increasing the use of the substrate.
- Maintaining good conductivity and prolonging the life of materials. Consequently, improving the performance of the membrane and electrode
- The ability to continue operating even when the pH, temperature, or wastewater content varies is referred to as "stable operation." Consequently, stability is maintained.

4.3 Overview of Optimization Methods

Optimization techniques have revolutionised scientific and technical applications by increasing the reliability and efficiency of systems. Optimization is essential in Microbial Fuel Cells (MFCs) due to the complicated interactions between biological, chemical, and electrochemical processes. Protons, electrons, and ultimately electrical energy are produced by the breakdown of organic substrates by microbial biofilms in MFCs. MFC efficiency is often limited by problems such as low substrate conversion rates, inadequate microbial activity, and inefficient electron transport. Optimization can solve these challenges by fine-tuning important parameters like substrate concentration, microbial community structure, and electrode material.

There are two main categories into which MFC optimization strategies can be divided:

4.3.1 Conventional optimization Algorithms:

Heuristic and gradient-based techniques are examples of conventional optimization techniques. Although gradient-based approaches are computationally effective and appropriate for problems involving continuous, differentiable objective functions, they frequently encounter difficulties when dealing with the non-linear, multi-modal issues that are common in MFC systems.

4.3.2 Nature-Inspired Optimization Algorithms:

These algorithms are very good at solving high-dimensional, complicated, non-linear problems since they are modelled after biological and natural processes. Gradient-Based Optimization (GBO), Grey Wolf Optimization (GWO), Particle Swarm Optimization (PSO), and Genetic Algorithm (GA) are a few examples.

Since each of these approaches has particular advantages and disadvantages, they can be applied to various MFC optimization scenarios

4.4 Gradient-Based Optimization

4.4.1 Fundamentals of Gradient-Based Methods

The computation of derivatives (gradients) of an objective function with respect to decision variables (such as electrode spacing, flow rate, and pH) is the foundation of gradient-based optimization techniques. Common gradient-based algorithms include conjugate gradient, steepest descent, and quasi-Newton methods, and they are most appropriate for problems in which the objective function is smooth and differentiable [44].

A traditional optimization method called gradient-based optimization (GBO) uses an objective function's gradient in relation to its variables to identify the best solutions. By directly utilising the mathematical structure of the problem, GBO places an emphasis on accuracy and efficiency in contrast to metaheuristic techniques, which prioritise exploration and unpredictability. It is particularly useful for convex optimization problems where the goal function is smooth and differentiable [39].

4.4.2 Gradient-Based Optimization (GBO) with Limited-Memory Broyden-Fletcher- Goldfarb-Shanno (L-BFGS-B)

For large-scale optimization problems with bound constraints, the Limited-Memory Broyden-Fletcher-Goldfarb-Shanno with Box Constraints (L-BFGS-B) approach is a sophisticated gradient-based optimization methodology. L-BFGS-B is computationally efficient for high-dimensional problems because it approximates the inverse Hessian matrix using a limited-memory technique, in contrast to conventional gradient methods. Box constraints are also included, which are essential for guaranteeing that variables stay within predetermined bounds throughout optimization [43].

L-BFGS-B is especially helpful in the context of Microbial Fuel Cells (MFCs) for optimising operational parameters like substrate concentration and microbial activity while making sure these parameters stay within reasonable physical bounds.

4.4.3 Recent Studies on Gradient-Based Optimization

Gradient-based techniques for MFC optimization have been effectively applied in a number of post-2020 studies, mostly under carefully monitored laboratory settings:
A 2021 study used a gradient-based technique to optimize substrate flow rate and HRT in a single-chamber MFC, resulting in a 25% increase in power density while preserving stable COD removal [47]. Another recent research in 2022 used gradient-based algorithms to fine-tune pH setpoints and external resistor values in real time, demonstrating a 15% power gain compared to fixed-parameter operation [48].

4.4.4 Mathematical Formulation

- **Objective Function:**

The optimization problem is expressed as:

$$\min_{\vec{x}} f(\vec{x}) \qquad (8)$$

subject to $\vec{l} \leq \vec{x} \leq \vec{u}$,

where $\vec{x}$ is the vector of decision variables, $f(\vec{x})$ is the objective function, and $\vec{l}$ and $\vec{u}$ are the lower and upper bounds, respectively.

- **Gradient and Approximation:**

The gradient of $f(\vec{x})$, $\nabla f(\vec{x})$, is used to iteratively update the variables:

$$\vec{x}^{k+1} = \vec{x}^{k} - \alpha_k \cdot \nabla f(\vec{x}^{k}) \qquad (9)$$

Here, α_k is a step size determined through line search. L-BFGS-B approximates the inverse Hessian matrix using limited-memory techniques to reduce computational overhead.

- **Handling Box Constraints:**

At each iteration, variables are projected back into the feasible region defined by $\vec{l}$ and $\vec{u}$:

$$\vec{x}_i = \max(\vec{l}_i, \min(\vec{x}_i, \vec{u}_i)) \qquad (10)$$

- **Stopping Criteria:**

The process continues until the gradient magnitude becomes sufficiently small ($\|\nabla f(\vec{x})\|<\epsilon$\|) or the maximum number of iterations is reached.
Some of the advantages of GBO are as follow. One being it's effectiveness in large scale problems. The limited-memory method is appropriate for high-dimensional MFC models since it lessens the computational load. The other being it's boundary restriction. Increases the dependability of findings by making sure that variables stay within reasonable bounds. Third it's ability to rapid convergence.Offers quick convergence rates along with the accuracy of gradient-based techniques.

Although it has several advantages but it do have some limitation. One it get stuck in local optima. In complicated, non-linear MFC systems, these techniques are particularly prone to becoming trapped in local optima. Secondly it dependency on the differentiability.Calculating gradients is made more difficult by the fact that many MFC performance functions entail discrete changes (such as biofilm separation). Third it computational cost. Numerical computation of gradients can be computationally demanding for large parameter spaces [49].

4.5 Genetic Algorithm (GA) Optimization

4.5.1 GA Foundations and Mechanisms

The Genetic Algorithm (GA) is an optimization method inspired by nature and founded on the ideas of evolution and natural selection. In order to solve complicated optimization problems that are otherwise challenging to handle with traditional methods, John Holland created it in the 1970s. GA works by using the processes of crossover, mutation, and selection to evolve a population of viable solutions over many generations. These evolutionary processes examine the search space for the best answers by simulating biological reproduction and mutation. Natural selection and genetics serve as the inspiration for Genetic Algorithms (GAs), population-based, metaheuristic optimization techniques [51]. A population of possible solutions, or individuals, encoded as chromosomes, is the starting point for a GA. The population changes as a result of repetitive processes of crossover, mutation, and selection; ideally, this convergence leads to optimal solutions.

In GA, a fitness function that measures the quality of each solution is used to assess the initial population of candidate solutions, known as chromosomes. The best solutions are chosen to procreate, bringing diversity (through mutation) and merging their traits (via crossover) to create the following generation. Until a stopping criterion—such as a maximum number of generations or convergence to an ideal solution—is satisfied, this iterative process keeps going.

4.5.2 Key steps in a GA:

- **Initialisation:**

Create a starting population that is either randomly selected or somewhat heuristic.

- **Evaluation:**

Determine each person's fitness, such as power density in an MFC setting.

- **Selection:**

Pick parents who are more suited to procreate.

- **Crossover:**

When parents exchange genetic material, kids are created.

- **Mutation:**

To preserve genetic variation, randomly change a few offspring genes.

- **Replacement:**

Create the following generation and carry on until the stopping or convergence requirements are satisfied.

4.5.3 Recent Advances in GA Optimization:

After 2020, GA research has investigated hybrid models and enhanced operators. The main research on Multi-objective GAs (MOGA). Power output is balanced with other goals, such as cost or effluent quality[55]. The second main advance is on adaptive mutation. In order to prevent premature convergence, adaptive mutation refers to mutation rates that vary dynamically depending on population variety [56]. The other main research being on parallel GAs. Making use of parallel computing to expedite assessments in large-scale MFC systems, particularly in the context of computational fluid dynamics (CFD) models [57]. The other main research being carried on Hybrid GA**.** In order to fine-tune solutions, hybrid GA combines GA with local search techniques such as gradient-based refinements [58].

4.5.4 GA Applications in Parameter Tuning for MFCs

GAs have been used in MFC optimization to determine the ideal external resistance, substrate feeding rate, and electrode spacing, among other characteristics. The fitness function gauges the overall performance of the MFC (e.g., maximum power density or COD removal efficiency), and researchers frequently store these characteristics in a structure resembling a chromosome [52]. In 2020, for instance GAs were used to optimize the carbon-to-nitrogen ratio in synthetic wastewater that was fed into an MFC. Membrane fouling was decreased and power density increased by 30% as a result of the optimized ratio [53]. Another study conducted in 2021 combined real-time sensor data (temperature, pH, and COD levels) with a GA-based controller that was able to dynamically modify operational settings and maintain a steady power output for 20 days [54]. Since GA can navigate complex, non-linear parameter spaces, its use in MFC optimization has grown significantly. A number of interrelated factors, including electrode spacing, biofilm characteristics, and substrate concentration, affect MFC performance. Researchers can find ideal combinations that optimize substrate conversion efficiency, power density, and current output by utilising GA.

The Genetic Algorithm has several advantage. One being it's robustness. GA is quite good at addressing non-linear and multi-modal issues. The other being it flexibility. It is appropriate for optimising a variety of MFC parameters because it can handle both continuous and discrete variables. One it's main capability to search globally. For complicated systems like MFCs, GA's ability to avoid becoming stuck in local optima is especially beneficial.

Although Genetic Algorithm have many advantages yet it has some limitation. One being it's computational intensity. Due to its iterative nature, GA can be computationally costly, especially when dealing with high-dimensional issues and huge populations. One of it's limitation being it's sensitivity to parameters settings. The effectiveness of GA is dependent on a number of parameters, including crossover probability, mutation rate, and population size, all of which must be carefully adjusted.

4.6 Particle Swarm Optimization (PSO) in MFCs

4.6.1 Fundamentals of PSO

Another population-based metaheuristic that draws inspiration from fish schools and bird social behaviour is Particle Swarm Optimization (PSO) [61]. Every potential solution is a "particle" that moves around the search space based on its own and its neighbours' experiences. Based on the individual (pbest) and global (gbest) best solutions discovered thus far, the algorithm modifies particle locations and velocities.

A bio-inspired optimization system called Particle Swarm Optimization (PSO) imitates the social behaviour of fish schools or flocks of birds. PSO was created by Kennedy and Eberhart in 1995, and because of its ease of use, adaptability, and effectiveness in resolving complicated and non-linear optimization issues, it has grown to be one of the most widely used heuristic optimization techniques [62]. PSO is perfect for solving multi-dimensional and non-differentiable objective functions since it does not rely on gradient information like conventional optimization methods do.

In PSO, a swarm of particles, representing alternative solutions, traverses the search space to reduce or maximize an objective function. Each particle has a position and velocity, which are iteratively updated based on its own experience and the experience of the entire swarm. Until a predetermined termination criterion—such as a maximum number of iterations or convergence to a particular solution—is satisfied, the process keeps going.

4.6.2 Key parameters in PSO:

- **Inertia Weight (ω\omega):**

Determines how much of the prior velocity is maintained

- **Acceleration Coefficients (c_1,c_2):**

Weights that balance the influence of personal and global best;

- **Population Size:**

The total number of particles in the swarm.

4.6.3 Mathematical Representation of PSO

The PSO algorithm is mathematically governed by two key equations:

4.6.3.1 Velocity Update Equation:

$$v_i^{k+1} = wv_i^k + c_1r_1(p_i^k - x_i^k) + c_2r_2(g^k - x_i^k) \quad (11)$$

Here:

- $\boldsymbol{v_i^k}$: Velocity of particle iii at iteration k.
- w: Inertia weight, which balances exploration and exploitation.
- c_1c_2: Cognitive and social coefficients that influence the particle's self-confidence and cooperation with neighbors.
- r_1r_2: Random numbers uniformly distributed between 0 and 1.
- p_i^k: Best position found by particle iii (personal best).
- g^k: Global best position identified by the entire swarm.
- x_i^k: Current position of particle i.

4.6.3.2 Position Update Equation:

$$\boldsymbol{x_i^{k+1} = x_i^k + v_i^{k+1}} \quad (\mathbf{12})$$

This equation updates the position of each particle based on its current velocity.

4.6.4 Recent Research

PSO's capacity to identify near-optimal solutions with fewer function evaluations is highlighted in a number of post-2020 comparative studies with other metaheuristics [65]. However, if particle swarm diversity is not preserved, PSO might occasionally converge too soon. To address this problem, hybridisation strategies have been put forth, such as combining PSO with mutation operators or random re-initialization [66].

For some types of continuous optimization problems, especially those with smoother objective functions or fewer constraints, PSO can be more computationally efficient than GAs [67]. However, PSO may need other techniques like inertia weight scheduling or multi- swarm approaches for extremely non-linear or multi-modal challenges in MFC design.

4.6.5 Implementing PSO for MFC Performance Enhancement

Similar to GAs, PSO has been used more and more for parameter tuning in MFC systems because it may converge rapidly and frequently requires less parameter sets [62]. In a 2020 study, for instance, PSO was used to optimize the geometry of a dual-chamber MFC, including the electrode arrangement and shape, which resulted in a 20% increase in power density over a baseline design [63]. Another study from 2022 showed that PSO could respond to changes in influent COD and temperature by efficiently controlling external resistance and pH setpoints in real-time [64].

4.6.6 Application in MFC Optimization

PSO's capacity to effectively manage complex, non-linear optimization issues makes it especially well-suited for parameter optimization in microbial fuel cells (MFCs).
Performance in MFCs is greatly impacted by crucial parameters such external resistance, microbial activity, and substrate concentration. The non-linearity of the underlying equations makes it difficult for traditional approaches to optimize various parameters concurrently. By using a population-based strategy to thoroughly explore the solution space, PSO gets over these restrictions.

4.6.7 PSO Workflow

The following steps are how the PSO algorithm works:

- **Initialisation:**

The positions and velocities of a swarm of particles are set at random. Each particle's objective function is assessed in order to ascertain the global best (g) and initial personal best (p_i).

- **Velocity Update:**

The velocity update equation is used to update each particle's velocity.

- **Position Update:**

The position update equation is used to update each particle's position.

- **Evaluation:**

Every particle undergoes a new evaluation of the objective function. If a better solution is discovered, the best positions on a personal and global level are updated.

- **Termination:**

Until a termination requirement is satisfied, the procedure is repeated.

The Particle Swarm Optimization has several advantage. One being it's scalability. PSO is appropriate for a variety of MFC configurations since it excels at solving optimization problems of all sizes. The other it's capability to search globally. To prevent premature convergence to local optima, the algorithm effectively searches the whole search space. One of the main advantage of PSO is being it's simplicity. PSO is a desirable option for real-time optimization jobs due to its simple implementation.

Although PSO has many benefits, PSO has many drawbacks. One being it's premature convergence. If swarm variety is not preserved, particles may converge too soon, especially on high-dimensional problems. Other being it's sensitivity to parameters. PSO performance is extremely sensitive to the selection of parameters, including learning factors (c_1, c_2) and inertia weight (w). The main drawback is it's computational overhead. PSO can become less effective in problems involving extremely complicated objective functions, despite being less computationally demanding than some optimization techniques.

4.7 Grey Wolf Optimizer (GWO)

4.7.3 Conceptual Introduction to GWO

A more recent metaheuristic, the Grey Wolf Optimizer (GWO), was motivated by the hunting habits and social structure of grey wolves [71]. GWO imitates a wolf leadership structure:

Alpha (α): The best solution found thus far.
Beta (β): The second-best option is beta (ββ).
Delta (δ): The third-best answer.
Omega (ω): The remaining population solutions.

α, β, and δ direct the search process, and the wolves adjust their placements in response to these top positions, convergently approaching the optimal solution.
The social structure and hunting habits of grey wolves in the wild served as the inspiration for the metaheuristic optimization technique known as "Grey Wolf Optimization" (GWO). GWO, which was proposed by Mirjalili et al. in 2014, solves complicated optimization issues by

imitating the cooperative tactics and leadership hierarchy found in wolf packs [72]. GWO's simplicity, adaptability, and efficiency in exploring and utilising the search space have led to its widespread use in a variety of fields. The population of GWO is separated into four groups, each of which represents a distinct role in the hierarchical structure of a wolf pack: alpha (α), beta (β), delta (δ), and omega (ω). While the β and δ wolves help lead the pack, the α wolves direct the search by preserving the best solutions. To ensure variation, the wolf packs follow and explore the search area.

4.7.4 Mathematical Representation of GWO

The GWO algorithm is based on three primary phases of wolf hunting behavior: encircling prey, hunting, and attacking prey. These behaviors are mathematically represented as follows:

- **Encircling Prey:**

$$\vec{\boldsymbol{D}} = | \vec{\mathbf{C}} \cdot \overrightarrow{\boldsymbol{X_p}} - \vec{\mathbf{X}} | \quad (\mathbf{13})$$

$$\vec{\boldsymbol{X}}\ (\boldsymbol{t}+\mathbf{1}) = \boldsymbol{X}\vec{\boldsymbol{p}} - \vec{\boldsymbol{A}} \cdot \vec{\boldsymbol{D}} \quad (\mathbf{14})$$

Here:

- $\vec{X}$: Current position of the wolf.
- $\vec{X}_p$: Position of the prey.
- $\vec{A}$,$\vec{C}$: Coefficients controlling exploration and exploitation.

- **Hunting:**

  The positions of the three best wolves (α, β, and δ) guide the search:

$$\vec{\boldsymbol{X}}(\boldsymbol{t}+\mathbf{1}) = \frac{\overrightarrow{\boldsymbol{X_1}}+\overrightarrow{\boldsymbol{X_2}}+\overrightarrow{\boldsymbol{X_3}}}{\mathbf{3}} \quad (\mathbf{15})$$

where $\vec{X}_1$, $\vec{X}_2$, and $\vec{X}_3$ are updated positions based on α, β, and δ.

- **Attacking Prey:**

  When $|\vec{A}|<1$ wolves converge on the prey, transitioning from exploration to exploitation.

4.7.3 Application in MFC Optimization

GWO is especially useful for optimising microbial fuel cell (MFC) parameters because of its capacity to achieve a balance between exploration and exploitation. GWO was used in this work to optimize substrate concentration (S), microbial activity (X_a), and other crucial factors in order to maximise the current output (I_{MFC}).

Due to its ease of use and strong worldwide search capabilities, GWO has started to be used in MFC research around 2020. For instance, in a 2021 study, a pilot-scale MFC treating industrial wastewater employed GWO to optimize a range of parameters, including temperature, external resistance, and substrate concentration, to maximise power density and substrate removal efficiency at the same time [72]. The findings demonstrated that GWO performed better than GA and PSO in achieving a better balance between COD removal rates and power production. In order to optimize the geometry of air-cathode MFCs, a hybrid GWO (with random restart) was used in another 2023 study. The results showed a 28% increase in power production over baseline designs [73].

4.7.4 GWO Workflow

- **Initialisation:**

Set the wolves' locations in the search space at random.

- **Fitness Assessment:**

Determine each wolf's level of fitness and update their αα, ββ, and δδ places.

- **Position Update:**

Utilising the hunting and surrounding formulae, update the wolves' locations.

- **Termination:**

Continue until the specified condition is satisfied, such as the maximum number of iterations or the convergence of the solution.

The Grey Wolf Optimization has several advantage. One being it’s fast convergence speed. Due to its balanced exploration and exploitation, GWO frequently converges swiftly in its early stages [74]. Other being it’s fewer parameters. Compared to GA or PSO, GWO is easier to operate because it requires fewer algorithmic parameters to be adjusted. One of it’s main advantage is it’s robust exploration. One of the issue being resolved by GWO is premature convergence. Premature convergence is less likely thanks to GWO's hunting and encircling strategies, which preserve diversity in the search space [75]. Also main advantage of GWO is it's ability to adapt. Depending on the complexity of the challenge, GWO can modify its search behaviour thanks to the dynamic coefficient.

4.8 Implementation of Optimization Techniques in MFC Systems

A crucial first step in raising the effectiveness and performance of Microbial Fuel Cell (MFC) systems is the application of ptimization techniques. This section describes how the MFC system model incorporates several ptimization techniques, including Grey Wolf Optimization (GWO), Particle Swarm Optimization (PSO), Genetic Algorithm (GA), and Gradient-Based Optimization (GBO). Enhancing MFCs' existing production and operational efficiency while resolving system limitations and difficulties is the main objective.

4.8.1 Numerical Simulation Framework

The numerical simulations were conducted using a mathematical model of MFCs, incorporating key dynamics such as substrate consumption, microbial growth, and electron transfer. This model served as the objective function for optimization. The parameters considered for improvement included:

- Substrate concentration (S)
- Active microbial population (Xa)
- Maximum microbial activity (Xm)
- Oxygen availability (M_ox)
- Current output (I_MFC)

The goal of the optimization was to preserve practical operating conditions while increasing the current output.

4.8.2 Objective Function and Limitations

A multi-variable objective function obtained from the MFC system's mathematical model served as the basis for the optimization algorithms:

$Objective\ Function:\ Maximize\ I_{MFC}(t) = f(S, X_a, X_m, M_{ox})$

Subject to constraints:

- Substrate concentration S:$S_{min} \leq S \leq S_{max}$
- Microbial population X_a: $X_{a\,min} \leq X_a \leq X_{a\,max}$
- Oxygen concentration M_{ox}: $M_{ox\,min} \leq M_{ox} \leq M_{ox\,max}$

  These constraints ensured that the optimization stayed within the practical limits of MFC operation.

4.8.3 Optimization Techniques

- **Gradient-Based Optimization (GBO)**

To compute gradients, GBO was used in conjunction with numerical differentiation. In order to maximise the objective function, the algorithm iteratively changed the parameters.
The two most important key parameters are convergence tolerance (ϵ) and step size (α).
The implementation of GBO required cautious initialisation to prevent local optima because it had trouble with non-linear, non-differentiable regions.

- **Genetic Algorithm (GA)**

GA started with a population of solutions and developed by crossover, mutation, and selection. The fitness function that was assessed I_{MFC}.The important key parameter for GA are The size of the population, the rate of mutation, and the likelihood of crossover are important parameters. It advantage over other techniques being Global optimization efficiency was improved by GA's resilience in navigating intricate, multi-modal search landscapes.

- **Particle Swarm Optimization (PSO)**

PSO used global and personal best positions to change each particle's position and velocity in the search space. The important key parameters of PSO are The inertia weight (w), cognitive coefficient (c1), and social coefficient (c2) are the three main parameters. It’s advantages over techniques being it fast convergence in the early phases cut down on computing time, which was a unique feature.

- **Grey Wolf Optimization (GWO)**

To balance exploration and exploitation, GWO modelled a hierarchy of wolves (alpha, beta, delta, and omega). The important key parameters of GWO are it's Pack hierarchy, search agent count. It's advantage over other technique being It was appropriate for dynamic MFC systems because to its adaptability and capacity to manage non-linear limitations.

4.8.4 Computational Experiments

To guarantee a fair comparison, each algorithm was evaluated using the same MFC model and the same initial conditions. Over a predetermined period of time, the simulations were run, and the outcomes were noted for the following metrics:

- Maximum output of current (I MFC max)
- The overall increase in current output
- Time convergence stability between iterations
- Stability

Table 1 - Computational Experiments

Algorithm	Peak Current (mA)	Improvement (%)	Convergence Time (s)	Stability
GBO	54.71	27.55	0.34	Moderate
GA	59.31	38.30	2.15	Moderate
PSO	59.32	38.30	1.89	Moderate
GWO	64.40	50.14	2.67	High

4.8.5 Algorithmic Insights

- **Intialization Sensitivity**

While deterministic initialisation in GBO needed fine-tuning, random initialisation in GA and PSO offered more expansive search possibilities.

a. Computational Costs:

GA and GWO performed exceptionally well in managing complicated dynamics, although GBO was computationally efficient for smaller systems.

b. Stability:

Because to its balanced exploration-exploitation strategy, GWO showed the highest stabilit

Chapter 5 RESULTS

This chapter main focus is on result being obtained from the optimization techniques being applied on MFC. These optimization techniques are being applied on MFCs separately. The results being obtained from each of the optimization technique are being showed separately with the discussion on each of these graphs. Then a thorough comparative analysis of these optimization techniques are being done in order to get a clear picture of these techniques have affected the output performance of MFCs also the performance metrics of these techniques are being compared and being evaluated to see which technique suited best and what effect of these techniques will have on MFCs performance. Also due to the unique characteristics of each optimization technique we compare which optimization technique suited in what circumstances. We will start by the result obtained by each optimization technique separately then we will move to comparative analysis.

5.1 Gradient Based Optimization Technique:

Graph:

The Figure. 4 shows the current graph after the Gradient Based Optimization.

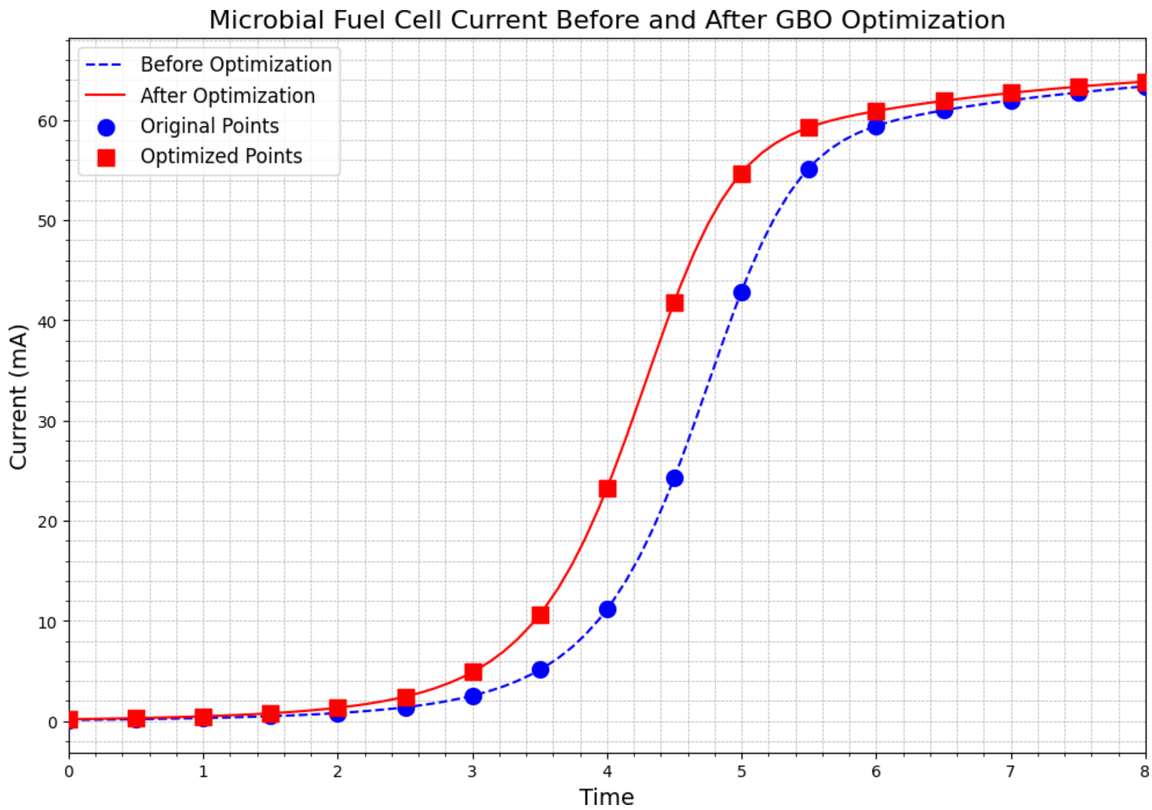

Figure 4 - Graph of GBO Optimization

- In comparison to the initial current (blue dotted line), the optimized current, shown by the red curve, rises quickly and smoothly.
- GBO reduces the delay seen in the unoptimized system by achieving a faster commencement of current rise.
- The optimized current of GBO approaches saturation more quickly, suggesting that the parameters have been tuned well to maximise MFC performance in the shortest amount of time.
- The GBO graph demonstrates its effectiveness in early-stage optimization by displaying a sharp rise in current during the first phase.
- The inaccuracy is greatly decreased as the optimized curve rapidly gets closer to the optimal trajectory.
- Following optimization, the points grow steadily and smoothly, demonstrating excellent precision and little variance.
- The significant improvement between 3.0 and 5.0 time units shows that GBO converges more quickly than other methods.
- The resulting current demonstrates GBO's superior performance in steady-state optimization by closely matching the theoretical maximum.

5.2 Genetic Algorithm Optimization:

Graph

The Figure. 5 shows the current graph after the Genetic Algorithm Optimization.

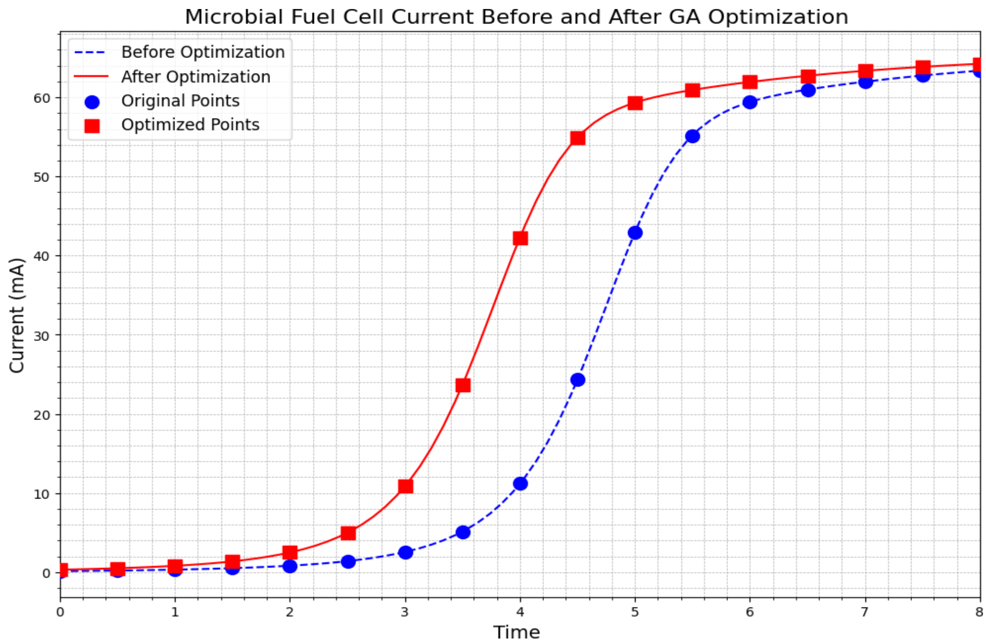

Figure 5 - Graph of GA Optimization

- Although the growth initially seems to be a little slower than GBO, the GA-optimized current (red curve) likewise shows a sharp increase in comparison to the original (blue dotted line).
- The technique's capacity to pinpoint and fine-tune important system characteristics is demonstrated by the evenly spaced red squares (optimized points) in the GA graph.
- GA optimizes the system for steady-state performance by ensuring a seamless transition to the saturation region.
- The resilience of GA in reaching convergence is demonstrated by the near overlap of the optimized curve with ideal current dynamics.
- Throughout all time intervals, the GA graph shows a consistent and slow increase in current.
- Although it moves a little more slowly than GBO in the first phase, the optimized curve shows a smooth transition.
- Although the trajectory is less aggressive, GA reaches final current levels that are comparable to those of GBO.
- This graph demonstrates GA's strong optimization capabilities, which make it dependable for applications that need incremental enhancements.

5.2.1 Particle Swarm Optimization

Graph:

The Figure. 6 shows the current graph after the Particle Swarm Optimization.

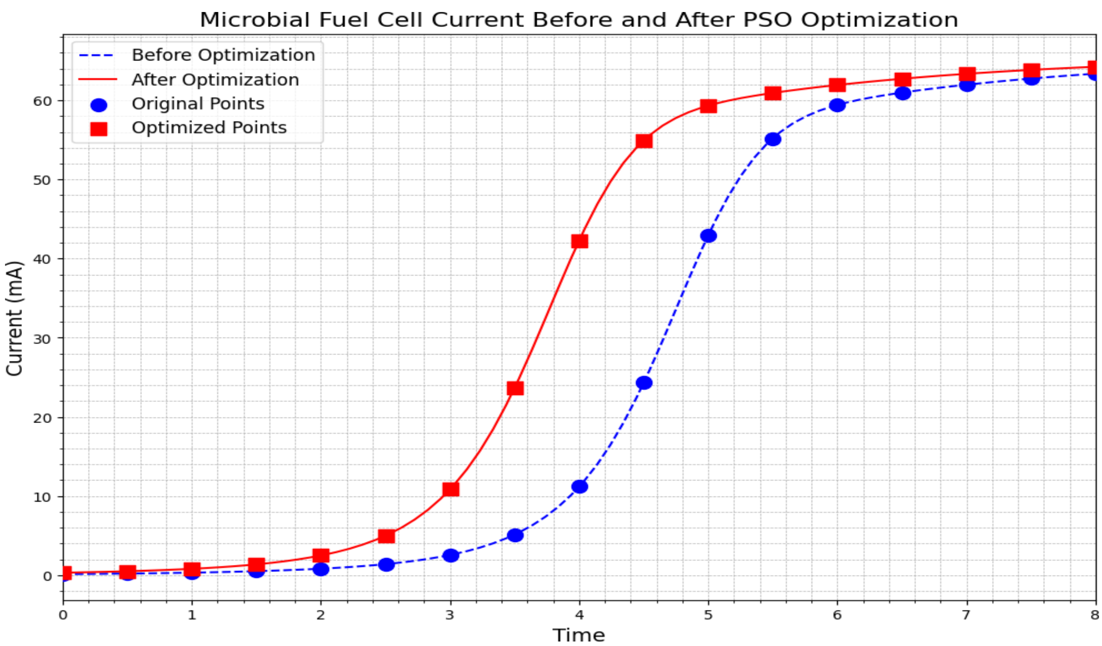

Figure 6 - PSO Optimization Graph

- The PSO-optimized current (red curve) shows a noticeable improvement over the original (blue dashed line).
- PSO's ability to make large adjustments during this phase is demonstrated by the red squares, or optimized points, which exhibit notable departures from the original locations during the mid-range.
- PSO quickly reaches greater current values, but when it gets closer to the steady-state zone, it exhibits a tapering effect.
- The red curve's smoothness illustrates how PSO balances stability and convergence speed during optimization.
- Although PSO does well in the intermediate phases, it is marginally less accurate than GBO and GA in terms of final alignment with ideal current values.
- During the middle time intervals (3.0–5.0 time units), PSO displays a noticeable improvement in current.
- When compared to the initial points, the optimized points in this phase show the most difference.
- In the mid-range, the curve shows a sharp increase, but as it gets closer to steady-state, it tapers off.
- In terms of steady-state accuracy, PSO trails GBO and GA by a small margin, even though the final optimized current is sufficient.
- The graph demonstrates PSO's ability to swiftly produce significant mid-range enhancements.

5.2.2 Grey Wolf Optimization

Graph

The Figure. 7 shows the current graph after the Grey Wolf Optimization.

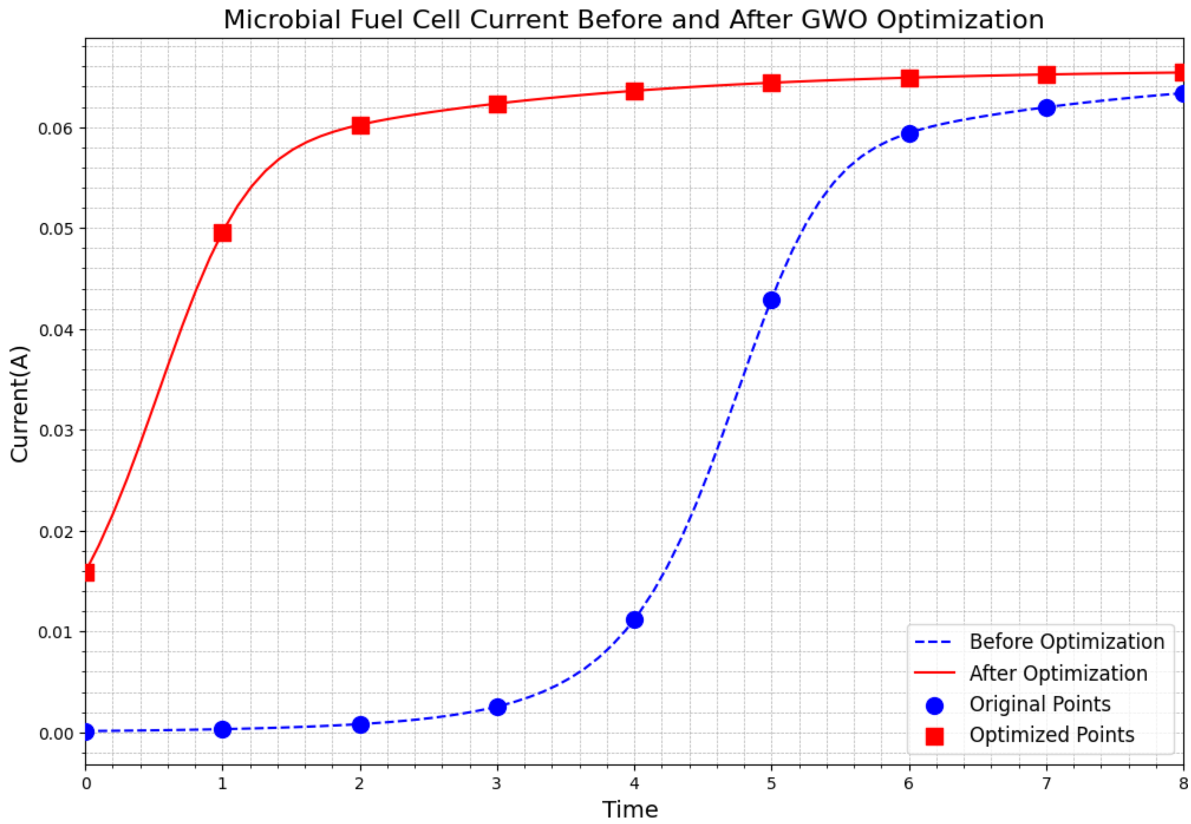

Figure 7 - GWO Optimization Graph

- The initial curve (blue dashed line) in the early phases is closely mirrored by the GWO-optimized current (red curve), which rises steadily and gradually.
- GWO's emphasis on accuracy over quick changes is demonstrated by the red squares, or optimized points, which show gradual gains over all time periods.
- After 6.0 time units, the optimized curve nearly resembles the ideal dynamics, demonstrating that GWO achieves minimum error in the steady-state area.
- The red curve's steady rise demonstrates how well GWO ensures accuracy and stability throughout optimization.
- For long-term optimization objectives, GWO is very effective because to its greater final precision, even though its initial progress is slower than that of GBO and PSO.
- The current increases gradually and steadily throughout all time intervals as a result of GWO optimization.

- A slower optimization procedure is reflected in the smaller discrepancies between optimized and original points as compared to other techniques.
- With optimized points that closely match the theoretical maximum, GWO delivers low error at the steady-state.
- The graph demonstrates GWO's accuracy later on, especially after 6.0 time units.
- Applications that value steady-state accuracy over quick early-stage advancements are best suited for this method.

5.3 Comparative Analysis of Optimization Techniques for MFCs

In order to overcome the difficulties that Microbial Fuel Cells (MFCs) present, like low power density, inefficient electron transmission, and limitations in substrate utilisation, optimization techniques are essential. By adjusting operating parameters, these methods seek to increase electrical production and boost system efficiency as a whole. The wide variety of optimization techniques includes deterministic techniques like Gradient-Based Optimization (GBO), which includes Limited-Memory Broyden-Fletcher-Goldfarb-Shanno with Box Constraints (L-BFGS-B), and metaheuristic algorithms like Genetic Algorithm (GA), Particle Swarm Optimization (PSO), and Grey Wolf Optimization (GWO). This section offers a thorough comparison of various methods, emphasising their computational effectiveness, performance measures, and applicability to MFC optimization.

Optimization methods are essential for improving microbial fuel cell (MFC) performance. These techniques tackle issues such as the non-linear relationships among internal resistance, biomass growth, and substrate utilisation. This study examines the efficacy of four optimization methods in MFC optimization: Grey Wolf Optimization (GWO), Particle Swarm Optimization (PSO), Genetic Algorithm (GA), and Gradient-Based Optimization (GBO).

5.3.1 Performance Trends

- **Gradient-Based Optimization (GBO):**

GBO is a traditional optimization technique that iteratively improves the objective function by relying on gradient information. It strength being laid in it’s

- Computationally effective for differentiable, small-scale systems.
- Implementation is simple.

It’s weakness being

- Restricted to functions that are smooth and differentiable.
- Challenges with multi-modal, non-convex problems, which are prevalent in MFCs.
- High probability of becoming stuck in local optima.

Performance Observations:

- Gradual yet steady increases in current output.
- Reaches its maximum at 54.71 mA, representing a 27.55% improvement overall.
- The absence of global search capabilities causes the optimization to stall later on.

- **Genetic Algorithm (GA):**

GA uses crossover and mutation mechanisms to evolve solutions while working on populations, drawing inspiration from natural selection. It strength being laid in it’s

- Strong performance for multi-modal, non-linear issues.
- Useful for investigating global optima.
- Able to manage multi-objective problems and limitations.

It’s weakness being

- Iterative population upgrades make it computationally costly.
- Later optimization phases show slower convergence.

Performance Observations

- It produces considerable gains, reaching a peak of 59.31 mA with an overall improvement of 38.3%.
- Steady performance over time, with a slight slowdown in the last phases.

- **Particle Swarm Optimization (PSO):**

PSO finds optima by simulating the social behaviour of particles travelling through a search space. It strength being laid in it’s

- Rapid convergence at first.
- Strong capacity for exploration.
- Computationally effective in contrast to GA.

It’s weakness being

- Prone to early convergence, particularly when dealing with multi-modal issues.
- Sensitive to changes in the parameters.

Performance Observations:

- Performance was comparable to GA, reaching a peak of 59.32 mA with a 38.3% overall improvement.
- Indicates sensitivity to tuning settings by displaying minor variations in optimization trends.

- **Grey Wolf Optimization (GWO):**

By striking a balance between exploration and exploitation, GWO imitates the social structure and hunting tactics of grey wolves. It strength being laid in it's

- Outstanding harmony between local refining (exploitation) and worldwide search (exploration).
- Strong management of dynamic systems and constraints.
- Computationally effective for dealing with big issues.

It's weakness being

Computational cost that is marginally greater than those of GBO and PSO.

Performance Observations:

Surpasses all methods with a 50.14% overall improvement and a peak current of 64.40 mA. Demonstrates remarkable early development (15,805% improvement) and sustains steady performance over time.

5.3.2 Performance Metrics Comparison

The following table summarizes key performance metrics for each optimization technique, including peak current, overall improvement, stability, and computational efficiency:

Table 2 - Performance Metrics Comparsion

Metric	GBO	GA	PSO	GWO
Peak Current (mA)	54.71	59.31	59.32	64.40
Overall Improvement (%)	27.55	38.30	38.30	50.14
Initial Growth (%)	58.45	154.85	154.85	15805.21
Stability	Moderate	Moderate	Moderate	High

Optimization Speed	Slow	Moderate	High	Very High

Observations:

- **GWO** achieves the highest peak current and overall improvement percentages, showing robust performance.
- **GA and PSO** deliver comparable results, with significant improvements but slightly lower consistency.
- **GBO** lags behind in both peak performance and overall improvement, making it less competitive for MFC optimization.

5.3.3 Improvement Trends Over Time

Table 3 - Improvement Trends

Time (Steps)	**GBO (%)**	**GA (%)**	**PSO (%)**	**GWO (%)**
Initial Phase	Moderate	High	High	Very High
Mid Phase	Steady	Steady	Slightly Fluctuating	Consistent
Late Phase	Tapers Off	Stable	Stable	Sustained Growth

- **GWO** exhibits exceptional initial growth due to its effective global exploration and fast convergence.
- **GA and PSO** show strong early growth but plateau in the later phase.
- **GBO** maintains slow, steady improvements but lacks impactful growth at any stage.

5.3.4 Adaptability and Scalability

Table 4 - Adaptability and Scalability

Criteria	**GBO**	**GA**	**PSO**	**GWO**
Adaptability	Limited	High	High	Very High

Scalability	Moderate	High	High	Very High
Computational Cost	Low	High	Moderate	Moderate

Observations:

- **GWO** successfully manages the complexity of MFC systems thanks to its remarkable flexibility and scalability.
- Although **GA** and **PSO** outperform **GWO** in many criteria, they require more computing power.
- Since **GBO** relies on smooth, differentiable objective functions, it is the least flexible.

5.3.5 Convergence Speed

GBO: With a sharp increase in current production in the early phases (up to 5.0 time units), GBO exhibits the fastest convergence. GBO is very effective for speedy optimization since the optimized curve moves swiftly to the saturation area.

GA: In contrast to GBO, GA exhibits a little slower convergence but keeps rising steadily. It maintains stability throughout the process by striking a balance between quick advancements and seamless transitions

PSO:In the mid-range (3.0–5.0 time units), PSO rises more quickly than GWO, but its initial adjustments are less forceful than those of GBO and GA. PSO works best in situations where a moderate rate of convergence is acceptable.

GWO: Although it has the slowest initial convergence, GWO is better suited for applications that need long-term stability since it prioritises accuracy through tiny, gradual increases.

5.3.6 Steady-State Performance

GBO: After optimization, it achieves outstanding steady-state performance and closely resembles the ideal curve. The small variations between the optimized and original numbers in the subsequent phases make this clear.

GA: it has smooth transitions and less oscillations, performing well in the steady-state zone. It offers a solid solution with steady-state behaviour that closely resembles GBO.

PSO: Although PSO greatly increases mid-range current production, its final steady-state performance shows minor departures from optimal values. This implies that its later-stage optimization could be improved.

GWO: Performs exceptionally well in steady-state accuracy, with very little error in the last phases. Superior alignment with the optimal current output is achieved through GWO's gradual but accurate changes.

5.3.7 Strengths and Weaknesses Comparison

Table 5 - Strength and Weakness

Technique	Strengths	Weaknesses
GBO	Simple to implement, computationally efficient.	Struggles with non-linear systems, prone to local optima, limited global exploration.
GA	Effective global search, handles multi-modal problems well.	Slower late-stage convergence, computationally expensive.
PSO	Fast initial convergence, strong exploration.	Prone to premature convergence, sensitive to parameter tuning.
GWO	Balanced exploration and exploitation, robust performance, excellent scalability.	Slightly higher computational cost compared to GBO and PSO.

Conclusions

The use of optimization approaches, such as Gradient-Based Optimization (GBO), Genetic Algorithm (GA), Particle Swarm Optimization (PSO), and Grey Wolf Optimization (GWO), to enhance the performance metrics of Microbial Fuel Cells (MFCs) was thoroughly examined in this study. The results highlight how important optimization is for improving important metrics including current output, substrate utilisation, electron transfer efficiency, and system stability as a whole. For optimization performance GWO show overall improvement of 50.14% and a peak current of 64.40 mA, GWO proved to be the most successful strategy. For the intricate, non-linear dynamics seen in MFC systems, its capacity to strike a balance between local refinement and global exploration makes it extremely effective. While GA and PSO with peak currents of 59.31 mA and 59.32 mA, respectively, and an overall improvement of 38.30%, both GA and PSO demonstrated strong performances. These techniques showed steady performance trends and robust initial growth, but their subsequent tapering improvements highlighted their vulnerability to premature convergence, GBO despite being simple to use and computationally efficient, GBO's application to non- linear, multi-modal issues that are typical of MFC systems was limited by its reliance on gradient information. With a total improvement of 27.55%, it produced the least amount of improvement in current output, peaking at 54.71 mA. Throughout all optimization phases, GWO showed the best stability, avoiding premature convergence and preserving steady trends. Due to their susceptibility to parameter adjustment, GA and PSO showed moderate stability but also slight variations during mid-phase optimization. GBO is less successful for larger, more complicated systems because of its low scalability and adaptability, which were demonstrated by its inability to maintain improvements past the initial phases. The study emphasises how optimization methods tackle basic issues with MFC functioning, including poor power density, substrate constraints, and inefficient electron transmission. To optimize system performance, advanced optimization techniques—especially those with strong global search capabilities—should be incorporated into MFC design and operating plans. The study's findings confirm the revolutionary potential of innovative optimization methods in raising MFC systems' performance. This study advances the development of effective, scalable, and sustainable energy solutions by tackling fundamental issues and outlining potential development paths. The incorporation of state-of-the-art optimization techniques into MFC systems will be essential to achieving global energy and environmental goals as the need for clean and renewable energy increases. In order to fully utilise MFC technology, this work is a fundamental first step. To overcome present obstacles and open the door for sustainable energy innovation, future developments will necessitate interdisciplinary cooperation, combining concepts from biology, computer science, engineering, and environmental science.

Future Work

Although this study offers important insight, it also opens up a number of directions for further investigation to improve the effectiveness and suitability of optimization methods in MFCs:

- Integration of Machine Learning

The accuracy and adaptability of optimization may be increased by utilising machine learning techniques like deep learning, reinforcement learning, or hybrid models.

Real-time system behaviour predictions and dynamic optimization parameter adjustments are made possible by these techniques.

- Optimization with Multiple Objectives

Multi-objective optimization should be the main focus of future research in order to improve several performance measures at once, including operational cost, environmental effect, and energy efficiency. Methods such as Pareto-based optimization may offer a fair way to satisfy a range of system needs.

- Hybrid Optimization Algorithms

Better performance may be attained by creating hybrid algorithms that combine the advantages of several approaches, such as GWO with GA or PSO. These hybrids provide efficiency and robustness by utilising the local refinement strengths of one approach and the global search capabilities of another.

- Analysis of the Economy and Environment

The effects of optimized MFC systems on the economy and environment should be taken into account in future research. Research evaluating sustainability, scalability, and cost-effectiveness will offer a more thorough grasp of these systems' viability for broad use.

Dynamic Systems Optimization

The adaptability of MFC technologies will be further increased by looking at the use of optimization approaches in dynamic and unpredictable environments, such as changing substrate concentrations or fluctuating energy need

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