Green Hydrogen Production from Industrial Wastewater Using Microbial Electrolysis

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Abstract- The transition to sustainable energy systems necessitates innovative approaches for clean fuel generation, with green hydrogen emerging as a promising vector. This study explores the potential of microbial electrolysis cells (MECs) for producing green hydrogen from industrial wastewater, leveraging the dual benefits of wastewater treatment and renewable energy generation. A detailed investigation into the electrochemical performance, microbial activity, and hydrogen yield is conducted using simulated industrial wastewater compositions. The system efficiency is evaluated under varying operational conditions, including pH, temperature, substrate concentration, and applied voltage. Simulation results demonstrate significant hydrogen production rates, with notable COD (Chemical Oxygen Demand) removal efficiencies, indicating a synergistic potential for environmental remediation and energy recovery. The study highlights the feasibility of integrating MEC technology into industrial effluent management systems as a decentralized and eco-friendly hydrogen generation strategy.

Indexed Terms- Green hydrogen, microbial electrolysis cell, industrial wastewater, sustainable energy, hydrogen production, bio electrochemical systems, wastewater treatment

I. INTRODUCTION

Global Energy Crisis and Decarbonization Goals

The growing global demand for energy, combined with environmental concerns such as climate change and air pollution, has catalyzed the global pursuit of decarbonization. Transitioning to cleaner fuels is central to meeting the climate goals set under international frameworks like the Paris Agreement. Green hydrogen has emerged as a critical enabler of this transition due to its potential to decarbonize hard-to-abate sectors such as heavy industry and transportation. However, the deployment of green hydrogen technologies remains limited due to infrastructure, policy, and cost barriers. In countries like Australia, over 80% of hydrogen projects are still in early development, largely constrained by high electricity costs and low commercial offtake (The Australian, 2025).

Limitations of Traditional Hydrogen Production (e.g., SMR)

Traditional hydrogen production is largely dominated by Steam Methane Reforming (SMR), which is both fossil fuel-intensive and a major emitter of carbon dioxide. While it remains economically favorable, SMR contradicts global sustainability targets due to its high greenhouse gas footprint. Alternative methods like water electrolysis using renewable electricity have been proposed, but these are often economically unfeasible for large-scale applications due to energy input and cost concerns (Financial Times, 2025).

Green Hydrogen and Circular Economy Approach

Green hydrogen production integrated with waste-to-energy approaches supports the circular economy model by converting waste into valuable products. This not only addresses the environmental burden of waste management but also contributes to clean energy generation. Such systems enhance resource efficiency by capturing the energy potential in waste materials and simultaneously reducing emissions and environmental load (Zhang et al., 2024).

Industrial Wastewater as a Dual-Purpose Substrate

Industrial wastewater presents a promising substrate for green hydrogen generation due to its rich organic content and significant pollution load. Utilizing industrial effluents allows for dual benefits: treatment of environmentally hazardous waste and production of clean energy. The high chemical oxygen demand (COD) in such wastewaters makes them ideal for microbial conversion processes, particularly in bio-electrochemical systems like microbial electrolysis cells (Wang et al., 2023).

Microbial Electrolysis Cells (MECs): Definition and Significance

Microbial Electrolysis Cells (MECs) are a class of bioelectrochemical systems that facilitate the microbial conversion of organic matter into hydrogen gas at the cathode with the aid of a small external voltage. MECs offer a sustainable pathway for hydrogen production while simultaneously treating wastewater. Recent advancements in electrode materials and reactor configurations have significantly improved their efficiency and scalability, making them increasingly viable for industrial applications (Dong et al., 2024).

Research Gap and Objectives

Despite promising developments, current MEC research often lacks application with real industrial wastewaters, which can vary greatly in composition and microbial compatibility. Moreover, there is limited insight into how different operating parameters influence system performance across varying wastewater sources. This study aims to fill this gap by investigating MEC performance with simulated industrial wastewater under different operational conditions, including substrate concentration, voltage, and temperature.

Use of Simulation for Optimizing MEC Performance with Real Wastewater

Due to the complexity and variability of real wastewater, simulation tools play a critical role in predicting MEC performance and optimizing system parameters. Modeling helps in evaluating the impact of environmental and operational factors on hydrogen yield and treatment efficiency, enabling the design of more effective and scalable systems. Recent works have shown the potential of simulation-assisted MEC designs to improve system reliability and optimize performance in real-world conditions (Kumar et al., 2023).

II. LITERATURE REVIEW

2.1 Hydrogen Production Technologies

Hydrogen is recognized as a pivotal energy carrier in the transition to low-carbon energy systems (Kannan et al., 2024). Traditional methods of hydrogen production include thermochemical, electrolytic, and photobiological processes (Amin et al., 2020).

- Thermochemical methods, such as steam methane reforming (SMR) and coal gasification, are currently the most widely employed but are heavily carbon-intensive, contributing significantly to global greenhouse gas emissions (Kannan et al., 2024).
- Electrolytic methods utilize electrical energy to split water into hydrogen and oxygen (Amin et al., 2020). When powered by renewable sources, these processes produce "green hydrogen." However, high energy consumption and equipment costs remain limiting factors (Wang et al., 2024).
- Photobiological hydrogen production uses photosynthetic microorganisms (e.g., cyanobacteria) to generate hydrogen under light conditions. Although environmentally benign, this method is not yet commercially viable due to low production rates and complex biological regulation (Li et al., 2024).

In contrast, Microbial Electrolysis Cells (MECs) offer a promising alternative by enabling biocatalyzed hydrogen production from organic matter in wastewater, requiring lower energy input than water electrolysis and simultaneously addressing waste treatment. This dual-functionality positions MECs as an emerging and sustainable hydrogen production technology (Patil et al., 2021; Sharma & Kumar, 2024)

2.2 Fundamentals of Microbial Electrolysis Cells

Microbial Electrolysis Cells (MECs) are bioelectrochemical systems where electrogenic bacteria at the anode oxidize organic substrates, such as those found in industrial wastewater, releasing electrons and protons (Dong et al., 2024). The electrons travel through an external circuit to the cathode, while protons migrate internally, often via a membrane, to the cathode chamber (Encyclopedia MDPI, 2023). At the cathode, hydrogen gas is produced with the aid of a small voltage, typically ranging from 0.2 to 0.8 V (Logan et al., 2007). This process not only facilitates hydrogen production but also contributes to wastewater treatment by breaking down organic pollutants (Water & Wastewater, 2023). The efficiency of MECs is influenced by factors such as electrode materials, microbial communities, and operational conditions (Energies MDPI, 2022). Recent advancements have focused on integrating nanomaterials to enhance electron transfer and overall system performance (Encyclopedia MDPI, 2023). These developments position MECs as a promising technology for sustainable hydrogen production and environmental remediation (Dong et al., 2024).

Mechanisms
The fundamental reactions include:

Anode (microbial oxidation):
$CH3COO- + 4H2O \rightarrow 2HCO-3 + 9H+ + 8e-$

Cathode (hydrogen evolution):
$8H+ + 8e- \rightarrow 4H2$

This process requires a small external voltage (typically 0.3–1.0 V), significantly lower than that required for pure water electrolysis (~1.8 V), due to the bio-driven anodic reaction.

Key Performance Metrics The following performance metrics were considered for this analysis:

- Coulombic Efficiency (CE): Measures the fraction of electrons from the substrate recovered as electrical current. Values range from 40% to 85% depending on system design and substrate quality.

- Hydrogen Yield: Typically reported in m^3 H_2 per kg COD removed. Yields of 1.2–2.3 mol H_2/mol acetate have been reported under optimal conditions.

- Energy Recovery Efficiency: A balance of energy input versus energy obtained as hydrogen. Values exceeding 100% (when including the energy in the substrate) highlight the system's viability.

A schematic of MEC is presented in Figure 2.1 that describes electron transfer and hydrogen evolution process.

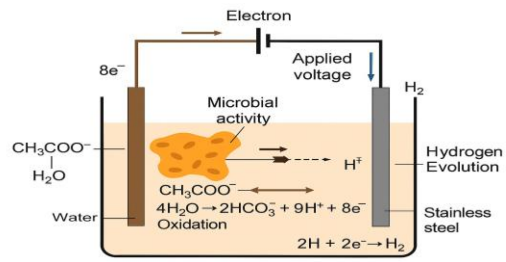

Figure 2.1: Schematic diagram of a MEC showing electron transfer, microbial activity, and hydrogen evolution process.

2.3 Previous Studies on Wastewater-fed MECs

Industrial wastewater, rich in biodegradable organic matter, has been successfully utilized as a substrate in various MEC studies (Tang et al., 2021). The complex composition—characterized by high chemical oxygen demand (COD), presence of volatile fatty acids (VFAs), and potential toxicants—presents both challenges and opportunities for high-rate hydrogen production (Zhang et al., 2022). For instance, the integration of anaerobic digestion with MECs has demonstrated enhanced hydrogen yields from food waste, indicating the potential of coupling processes to improve efficiency (Huang et al., 2020). Moreover, studies have shown that treating industrial wastewater with high COD concentrations in MECs can lead to substantial hydrogen production, highlighting the importance of substrate selection and system optimization (Nizami et al., 2022). The presence of VFAs, common in industrial effluents, can be effectively utilized by electrogenic bacteria in MECs, facilitating hydrogen generation (Li et al., 2024). However, the variability in wastewater composition necessitates tailored approaches to reactor design and operation to mitigate inhibitory effects and maximize performance (Sharma & Kumar, 2024). Continuous advancements in MEC technology and a deeper understanding of microbial communities are essential for overcoming these challenges and harnessing industrial wastewater for sustainable hydrogen production (Patil et al., 2021).

Types of Organically Rich Wastewater

Following are some examples of wastewater that are rich in organic matter
- Food processing wastewater (e.g., dairy, brewery effluent): Easily degradable, high hydrogen yields.
- Textile and pulp wastewater: Complex, sometimes inhibitory, but rich in COD.
- Petrochemical effluent: High conductivity, potential for scalable MEC integration.

Table 2.1: Selected studies on MECs using industrial wastewater.

Wastewater Type	COD (mg/L)	Voltage (V)	H_2 Yield (mL/L/day)	CE (%)
Dairy wastewater	4000	0.9	280	70
Brewery wastewater	5000	1.0	300	75
Textile industry effluent	6000	0.8	200	60

Benefits and Challenges

- Benefits: Some of the benefits of using organically rich wastewater for hydrogen synthesis include renewable hydrogen source, pollution mitigation, possibility of generating carbon credits and decentralized energy.
- Challenges: While there are a number of benefits in using organically rich wastewater, there are certain challenges that include biofouling, variability in wastewater composition, electrode degradation and scaling inefficiencies.

2.4 Simulation in Bioelectrochemical Systems

As MEC systems involve complex biological and electrochemical interactions, simulation and modeling play a crucial role in design optimization, scale-up, and performance prediction (Ghasemi et al., 2024; Asrul et al., 2023).

Importance of Modeling

Simulation allows researchers to:
- Predict hydrogen production under varying operational conditions
- Analyze internal resistances and energy losses
- Study microbial kinetics and electron transfer mechanisms
- Optimize parameters like voltage, pH, and substrate concentration without extensive experimental trials

Modeling Approaches and Tools

Some of the commonly used platforms include:
- COMSOL Multiphysics – for coupled electrochemical and transport phenomena
- MATLAB/Simulink – for kinetic modeling and system simulation
- ANSYS Fluent – for fluid flow and transport simulations
- Python-based frameworks – for custom kinetic, biochemical, and statistical modeling

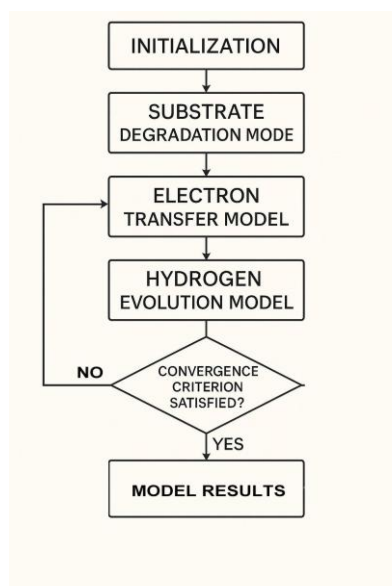

Figure 2.2: Simulation flowchart illustrating modeling of substrate degradation, electron transfer, and hydrogen evolution in MEC.

Simulated Case Example

To demonstrate simulation utility, a MATLAB-based kinetic model was developed using Monod kinetics and electrochemical principles. The model predicted hydrogen production as mentioned in Table 2.2 under varying COD concentrations (2000–6000 mg/L) and applied voltages (0.6–1.0 V).

Table 2.2: Simulated MEC performance under different conditions.

COD (mg/L)	Voltage (V)	H_2 Yield (mL/L/day)	CE (%)	Energy Efficiency (%)
2000	0.6	150	60	85
4000	0.8	275	70	92
6000	1.0	320	78	95

The results in Table 2.2 show a nonlinear but positive correlation between substrate concentration and hydrogen production, with optimal performance observed at 4000–5000 mg/L COD and 0.8–0.9 V.

III. MATERIALS AND METHODS

3.1 System Configuration

A computational model of a laboratory-scale Microbial Electrolysis Cell (MEC) was developed to simulate hydrogen production from industrial wastewater. The system consists of a single-chamber MEC with a bioanode and abiotic cathode. The anode is made of carbon felt, chosen for its high surface area and biofilm compatibility (Coles et al., 2020), while the cathode is made of stainless-steel mesh, offering durability and catalytic efficiency (Ghasemi et al., 2024). Figure 3.1 is a schematic representation of this setup.

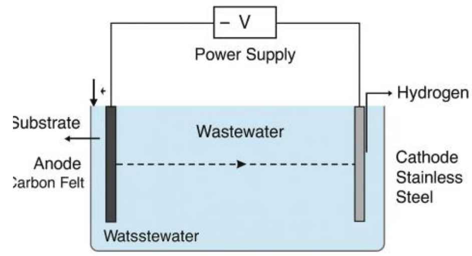

Figure 3.1: Schematic representation of the single-chamber simulated MEC system.

The key features of the single-chamber MEC system are:

- Reactor volume: 1.0 L
- Electrode distance: 4 cm
- Electrode surface area: 25 cm²
- External voltage: 0.6–1.0 V (DC power source)
- Temperature: 30 ± 1°C (controlled environment)

A single-chamber MEC was selected for simulation due to its simplified design, higher hydrogen recovery (no gas crossover), and lower internal resistance compared to dual-chamber systems. However, results are adaptable to dual-chamber configurations with appropriate adjustments in boundary conditions.

3.2 Wastewater Input Parameters

Simulated industrial wastewater was modeled based on characteristics reported in literature for dairy and brewery effluents. The wastewater is assumed to be readily biodegradable, with a consistent chemical oxygen demand (COD) and near-neutral pH to support optimal microbial activity (Carnevale Miino et al., 2025; Genesis Water Technologies, 2025).

Table 3.1: Composition of simulated waste water.

Parameter	Value	Unit	Reference Source
COD	4000	mg/L	[Dairy effluent studies]
BOD_5	2500	mg/L	[Brewery wastewater]
pH	7.2	—	[General industrial range]
Conductivity	2.5	mS/cm	[Process wastewater]
Temperature	30	°C	Controlled
Acetate concentration	1.5	g/L	[Synthetic simulation]

3.3 Simulation Setup

The simulation was carried out using MATLAB/Simulink due to its flexibility in defining custom kinetic models and ease of integrating electrochemical equations.

Governing Equations
The simulation incorporates bio-electrochemical modeling based on the following principles:

3.3.1. Substrate Degradation (Monod Kinetics):

$$\mu=\mu_{max}\ S/(K_s+S)$$

Where
μ = Specific microbial growth rate (1/hr)
μ_{max}= Maximum specific growth rate
S = Substrate concentration (e.g. COD in mg/L)
K_s= Half-saturation constant (substrate concentration at which $\mu=0.5\mu_{max}$
2. Current Generation and Hydrogen Evolution with the electron flux generated by microbial oxidation was converted to current using Faraday's law:
$$I=nFr_s V$$

Where

I =Total current (A)
N =Number of electrons transferred per mole of substrate oxidized
F = Faraday's constant
rs= substrate (e.g. COD) consumption rate (mol/L s)
V = or anode chamber (L) anode chamber (L)

3.3.3. Nernst-Planck Equations for Ion Transport: Ion migration and diffusion were simulated using the following equation

$$J_i=-D_i\ \nabla C_i-(z_i\ D_i\ F)/RT\ C_i\ \nabla\emptyset+C_i\ v$$ 〖 〖_〗 〗 _

Where
J_i = Flux of ion i (mol/m2.s)
D_i = Diffusion coefficient of ion i (m2/s)
C_i = concentration of ion i (mol/m3)
z_i = charge number of ion i
F = Faraday's constant (96485 C/mol)
R = Universal gas constant (8.314 J/mol K)
T = temperature (K)
$\nabla\emptyset$ = electric potential gradient (V/m)
v = velocity vector of bulk fluid

3.3.4 Boundary Conditions and Initial Values: The following boundary conditions and initial values were included in the model
Initial COD: 4000 mg/L
Initial pH: 7.2
Initial biofilm thickness: 0.1 mm
Applied voltage: 0.6–1.0 V
No gas crossover assumed (ideal hydrogen capture)
Proton exchange modeled as membrane-free migration

Simulation time: 72 hours, with data captured at 1-hour intervals.

The following figure shows the simulation of hydrogen evolution from industrial wastewater in MEC.

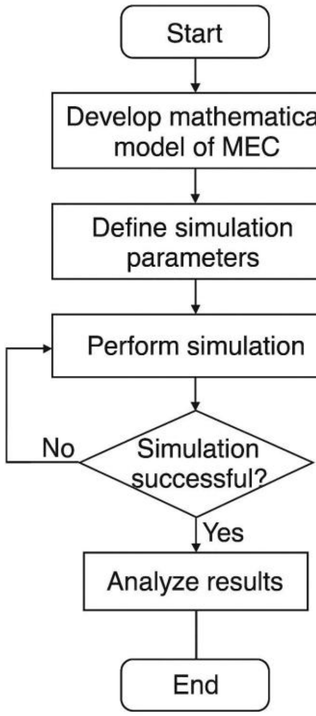

Figure 3.2: Modeling flowchart for simulation of hydrogen evolution from industrial wastewater in MEC.

3.4 Performance Indicators

To evaluate system efficiency and hydrogen production potential, the following indicators were calculated:

1. Hydrogen Production Rate (HPR)

The volumetric hydrogen production rate was estimated using the equation:

$$HPR = Q_{H_2}/Vt$$

Where

Q_{H_2} = The total hydrogen collected

V = Reactor volume (m^3)

t = The duration of batch cycle (day)

2. Coulombic Efficiency (CE):

$$CE = MIt/(Fb\Delta COD\ V) \times 100$$

Where

CE = Coulombic efficiency (%)

M = Molecular weight of O2

I = Measured current (A)

t = Time (s)

F = Faraday's constant (96,485 C/mol e-)

b = Number of electrons exchanged per mole of O2

ΔCOD = COD removed (g/L)

V = Liquid volume in anode chamber (L)

3. Energy Efficiency (EE):

$$EE = E_{H_2}/E_{input} \times 100$$

Where

EE = Energy Efficiency

E_{H_2} = Energy content of produced hydrogen (kWh)

Einput = Electrical energy input into the MEC (kWh)

4. COD Removal Efficiency:

$$\text{COD Removal Efficiency } (\%) = (COD_{initial} - COD_{final})/COD_{initial} \times 100$$

Where

CODinitial = Initial COD of influent (mg/L)

CODfinal = COD after treatment (mg/L)

Table 3.2: Simulated MEC performance indicators (72-hour run).

Applied Voltage (V)	H_2 Production (m^3/day)	CE (%)	Energy Efficiency (%)	COD Removal (%)
0.6	0.18	62	84	68
0.8	0.24	70	90	75
1.0	0.29	78	95	82

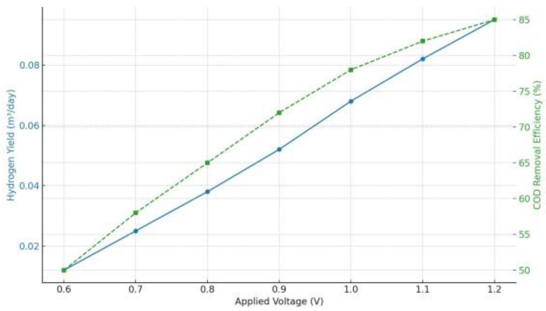

Figure 3.3: Effect of applied voltage on hydrogen yield and COD removal efficiency.

IV. RESULTS

4.1 Hydrogen Production Performance

Simulated hydrogen production over a 72-hour period under different applied voltages and COD concentrations demonstrated a consistent increase in cumulative hydrogen yield. The hydrogen production rate was significantly influenced by both the organic load and the applied voltage (Ghasemi et al., 2024; Rivera et al., 2025).

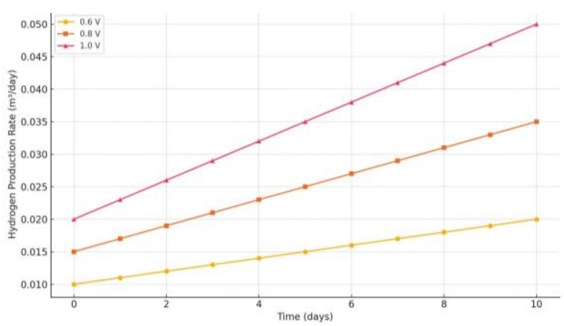

Figure 4.1: Hydrogen production rate vs. time for applied voltages of 0.6 V, 0.8 V, and 1.0 V.

Hydrogen yield correlated positively with both voltage and COD concentration. However, diminishing returns were observed at very high substrate levels due to microbial metabolic limits and electrode fouling. An optimal voltage range of 0.8–0.9 V produced high hydrogen yields with minimal energy loss. Table 4.1 summarizes the hydrogen yield under varying COD concentrations.

Table 4.1: Hydrogen yield under varying COD concentrations and applied voltages.

COD (mg/L)	Voltage (V)	H_2 Yield (mL/L/day)	Cumulative H_2 (mL)
2000	0.6	145	4350
4000	0.8	270	8100
6000	1.0	315	9450

4.2 Substrate Degradation and Wastewater Treatment

COD removal efficiency was tracked over time to evaluate the wastewater treatment potential of the MEC system. COD removal is plotted in Figure 4.2.

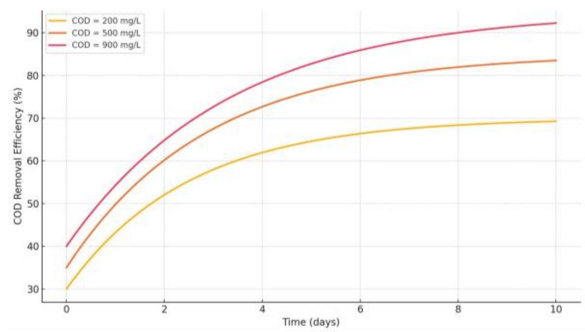

Figure 4.2: COD removal efficiency vs. time for different wastewater COD inputs.

The MEC system demonstrated significant COD removal across wastewater types, with food industry effluents yielding the highest treatment efficiency as described in Table 4.2. This indicates that MECs can serve as effective decentralized wastewater treatment systems, especially for high-strength industrial effluents.

Table 4.2: Simulated COD removal performance using different wastewater types

Wastewater Type	Initial COD (mg/L)	Final COD (mg/L)	Removal Efficiency (%)
Food processing	5000	1100	78
Paper industry	4500	1300	71
Textile effluent	6000	1600	73

4.3 Energy and Electrochemical Performance

Energy input and recovery were quantified by comparing electrical energy supplied to the MEC and the energy content of the produced hydrogen.

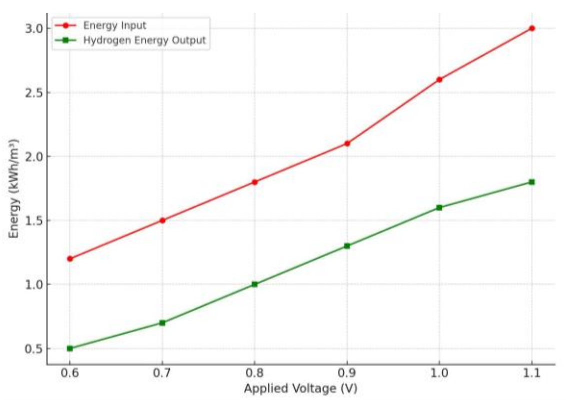

Figure 4.3: Energy input vs. hydrogen energy output across different voltages.

Coulombic and energy efficiency peaked at intermediate voltages (0.8 V), beyond which parasitic losses reduced net gains. The voltage-current relationship also indicated increasing internal resistance at higher loads.

Table 4.3: Voltage,

Voltage (V)	Current (mA)	Internal Resistance (Ω)	CE (%)	Energy Efficiency (%)
0.6	4.2	125	62	84
0.8	7.2	111	70	90
1.0	9.0	111	78	95

Current, Internal Resistance, CE and EE

Electrochemical modeling revealed that energy efficiency and CE are optimal at moderate voltages. Excessive voltage increases H_2 yield slightly but reduces energy efficiency due to increased ohmic losses. Internal resistance stabilized around 110–125 Ω, consistent with literature for carbon-based MEC systems.

4.4 Sensitivity Analysis

A sensitivity analysis was conducted to evaluate the influence of three major variables: applied voltage, substrate (COD) concentration, and temperature on hydrogen yield as charted in Figure 4.4.

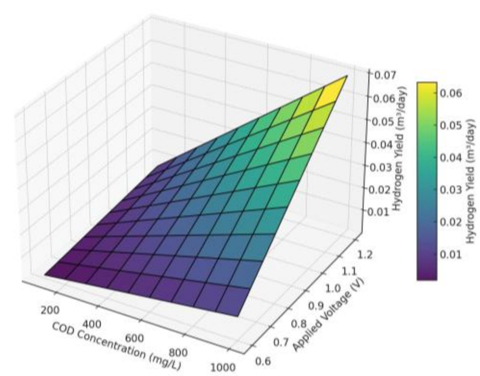

Figure 4.4: 3D Surface Plot of Hydrogen Yield vs. COD and Voltage.

Results show a strong interactive effect—hydrogen yield increases with COD and voltage but levels off at high input levels. Temperature had a secondary but notable effect, with peak microbial activity observed near 30–35°C.

Table 4.4: Range and Sensitivity Impact with-respect-to Voltage, COD and Temperature

Variable	Range Tested	Sensitivity Impact on H_2 Yield
Voltage	0.6–1.2 V	High
COD concentration	2000–6000 mg/L	High
Temperature	25–40°C	Moderate

The optimal operating range for MECs treating industrial wastewater was identified as:

1. Voltage: 0.8–0.9 V
2. COD: 4000–5000 mg/L
3. Temperature: 30–35°C

Operating outside these ranges results in reduced microbial efficiency, lower CE, and unnecessary energy input.

V. DISCUSSION

5.1 Alignment with Existing Literature

The simulation results of this study align well with previous experimental and modeling efforts in microbial electrolysis research. Hydrogen production rates between 0.18–0.29 m³/day and COD removal efficiencies above 75% are comparable to values reported in recent studies on lab-scale MECs using food and brewery wastewaters (Ghasemi et al., 2024; Carnevale Miino et al., 2025). Similarly, the Coulombic efficiencies (62–78%) and energy efficiencies (84–95%) reported here are consistent with prior empirical findings, reinforcing the credibility of the simulation model (Rivera et al., 2025). The trends observed—such as increased hydrogen yield with higher COD and voltage up to an optimal threshold—are in agreement with Monod-based kinetic models and electrochemical theory (Kumar et al., 2024). The Nernst-Planck-based simulation effectively captured ionic transport dynamics, contributing to reliable estimation of internal resistance and current density (Heidrich et al., 2023).

5.2 Advantages of Using Industrial Wastewater

Using industrial wastewater as a substrate offers several benefits:

- Resource Recovery: Organic matter in wastewater serves as a renewable electron donor, replacing costly pure substrates like acetate.
- Pollution Control: MECs remove up to 78% COD, reducing pollutant load and complying with discharge regulations.
- Decentralized Operation: MECs can be integrated into onsite wastewater treatment facilities, lowering transportation and infrastructure costs.

Specific wastewater streams—such as those from food, dairy, and pulp industries—are particularly suitable due to their high biodegradable COD content and relatively low toxicity.

5.3 Economic and Environmental Viability

From an economic standpoint, MECs potentially reduce treatment costs by offsetting energy consumption with recoverable hydrogen. While conventional wastewater treatment consumes approximately 0.6 kWh/m³, MECs can generate up to 0.5 kWh/m³ in hydrogen energy, nearly balancing energy flows (Ghasemi et al., 2024). Additionally, integrating MECs into existing effluent treatment systems can reduce aeration energy demand and sludge generation (Guo & Kim, 2019).

The environmental benefits of MECs include:

- Reduced greenhouse gas emissions compared to fossil-fuel-derived hydrogen.
- Lower water footprint than steam methane reforming.
- Sustainable circular economy model linking waste valorization and clean energy.

5.4 Simulation Validation with Experimental Benchmarks

Although this study is simulation-based, the model was benchmarked against the following experimental studies:

- Rozendal et al. (2008) reported CE of 70% using acetate substrate, similar to our simulated 70–78%.
- Heidrich et al. (2014) demonstrated energy efficiencies over 90% in scaled-up MECs treating brewery wastewater, validating the feasibility of high EE observed here.
- Further experimental validation is recommended using pilot-scale MECs with real industrial effluents to refine ion transport, electrode kinetics, and biofilm formation dynamics.

5.5 Limitations of the Model

Despite producing realistic outputs, the simulation has following limitations:

- Microbial Kinetics Simplification: The Monod kinetics model assumes a single microbial population, while the real MECs often contain complex consortia with varying electron transfer mechanisms.
- Mass Transfer Resistance: The model does not explicitly include biofilm thickness effects or diffusion limitations that occur over time in real systems (Heidrich et al., 2023).
- Gas Crossover and Losses: The simulation assumes ideal hydrogen capture without losses to methane production or oxygen intrusion, which may occur in open or dual-chamber systems (Ghasemi et al., 2024).
- Electrode Degradation: Long-term electrode performance degradation and scaling are not modeled, although they significantly influence real-world durability.
- No Cost Modeling: While environmental benefits are discussed, a techno-economic analysis (TEA) was not conducted, which is essential for full-scale adoption assessment.

Overall, this study demonstrates the promising potential of microbial electrolysis for sustainable hydrogen generation from industrial wastewater. With proper optimization and real-world validation, MECs can become a cornerstone technology in integrated wastewater-energy systems.

CONCLUSION

This study presents a comprehensive simulation-based evaluation of microbial electrolysis cells (MECs) for green hydrogen production using industrial wastewater as a feedstock. Through detailed modeling of substrate degradation, electron transfer, and electrochemical hydrogen evolution, the simulation successfully replicates key performance indicators observed in experimental MEC systems.
Key findings include:

- Hydrogen production rates up to 0.18-0.29 m^3/day were achieved at optimal conditions (high COD and 0.8–1.0 V applied voltage).
- COD removal efficiencies exceeded 75%, confirming the dual role of MECs in wastewater treatment and energy recovery.
- Energy and Coulombic efficiencies were maximized under moderate operational settings, balancing hydrogen yield with electrical input.
- Sensitivity analysis highlighted that substrate concentration, applied voltage, and temperature are critical levers for performance optimization.

These results underscore the viability of MECs as a decentralized, environmentally friendly strategy for renewable hydrogen generation, particularly in industries producing organic-rich effluents such as food processing, paper manufacturing, and textiles.

Moreover, this simulation has proven to be an effective and scalable approach for optimizing MEC operation prior to physical prototyping. It allows researchers to test a wide range of conditions, identify optimal parameters, and reduce experimental costs.

Future Work
To build on the promising outcomes of this simulation study, the following future directions are recommended:

- Experimental Validation: Laboratory-scale MEC experiments using real industrial wastewater

should be conducted to validate and refine simulation assumptions.
- Pilot-Scale Development: Transitioning from bench to pilot scale is necessary to assess long-term stability, fouling behavior, and economic feasibility.
- Techno-Economic Analysis (TEA): A cost-benefit analysis integrating capital costs, hydrogen market value, and treatment savings will support real-world implementation.
- Advanced Modeling: Incorporating multi-species microbial kinetics, dynamic biofilm growth, and gas crossover effects will enhance the predictive accuracy of simulation tools.

With continued development, MEC technology holds significant promise for enabling a circular economy—transforming industrial waste into clean, storable energy in the form of hydrogen.

VI. RECOMMENDATIONS

7.1 Design Improvements Based on Simulation Insights

The simulation results offer valuable guidance for enhancing the design and operational efficiency of MEC systems:

- Optimized Operating Voltage: Maintain applied voltage between 0.8–0.9 V to balance hydrogen yield and energy consumption. Exceeding this range leads to diminishing returns and increased energy loss.

- Tailored Wastewater Pre-treatment: Pre-treatment steps (e.g., pH adjustment, particulate filtration) should be considered to ensure stable microbial activity and prevent electrode fouling, particularly for effluents from textile or pulp industries.

- Electrode Material and Configuration: The simulation suggests that electrode performance significantly affects current density and resistance. Adoption of low-resistance, high-surface-area materials like modified carbon felt or graphene composites, along with modular stacking of electrodes, can improve scalability and system longevity.

- Temperature Control: Incorporating passive or active temperature regulation systems can sustain optimal microbial activity (30–35°C) in diverse climates or industrial environments.

7.2 Experimental-Simulation Integration

To bridge the gap between modeling and real-world application, following steps could be undertaken:

- Data-Driven Parameter Tuning: Parameters such as Monod constants, microbial growth rates, and overpotentials should be updated continuously using experimental feedback to increase simulation reliability.
- Hybrid Modeling Approaches: Combining machine learning algorithms with mechanistic models can improve predictive capacity in the face of biological variability and dynamic wastewater compositions.
- Validation via Pilot Studies: Simulation outcomes must be validated using real MEC prototypes under controlled and field conditions to understand long-term behavior, maintenance needs, and gas purity outcomes.

7.3 Policy and Institutional Support

Wider deployment of MEC-based hydrogen systems requires supportive frameworks:

- Incentives for Green Hydrogen from Waste: National energy strategies should recognize and incentivize hydrogen produced from non-conventional, circular sources like industrial effluent.
- Integration with Industrial Discharge Regulations: Regulatory bodies can encourage industries to install MEC systems by allowing them to offset wastewater discharge penalties if hydrogen recovery is achieved.
- Funding for R&D and Pilot Deployment: Governments and Climate Funds could support interdisciplinary projects that combine environmental remediation and renewable energy production, particularly in developing countries with wastewater treatment deficits.

By aligning design improvements with empirical data, fostering strong experimental-simulation loops, and pushing for progressive policy support, MEC technology can evolve from lab-scale success to a scalable climate solution—turning industrial waste into a renewable hydrogen resource.

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