Microbial Electrochemical Systems for Enhanced Wastewater Treatment and Energy Recovery

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ABSTRACT

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Narges Rahimi

Due to urbanization and population growth, wastewater generation and related energy consumption are still rising. In this regard, new technologies like bio-electrochemical systems (BESs) can play a significant role in simultaneously treating waste materials and energy recovery. In this research, three kinds of BESs, including single-chamber (SCMEC) and dual-chamber (DCMEC) microbial electrolysis cells and microbial fuel cells (MFC), have been examined as wastewater treatment pathways in urban areas. The mathematical modeling of the mentioned technologies is carried out, and the models are implemented using the Python programming language. The Radaue method as a numerical solution has been adapted to solve the ODE equations for such systems. The mathematical modeling results show a good agreement compared to previous works that used different numerical solutions such as ODE 15. The results show that the hydrogen production rate in SCMEC is less than in DCMEC because of hydrogenotrophic bacteria activities, which are reported as about 0.86 m^3 and 0.56 m^3 of H_2 gas per m^3 of wastewater, respectively. Also, the model analysis shows that applied potential and anode surface area directly affect hydrogen production rates SCMEC and DCMEC. The calculated electric energy output was 0.033 kWh per m^3 of wastewater has been found for the MFC. Two real case studies in Montreal have been considered to investigate the potential of using the mentioned systems on an urban scale. The first district, including residential buildings, has a total daily wastewater generation of 3,000 m^3/day, and 75 m^3/day is assumed for the second one with a smaller non-residential building project. Moreover, some comparisons between the research outputs and real data have been made to investigate the potential of applying the BESs as a wastewater treatment method. For instance, the energy consumption by BESs and wastewater treatment plants have been compared. Also, DCMEC and SCMEC have been compared against water electrolysis technologies for hydrogen production. In addition, the feasibility of using the generated hydrogen and power via microbial systems as fuel in green cars has been investigated as a final step.

Keywords: Wastewater treatment; Renewable energy; Microbial electrolysis cell; Microbial fuel cell; Mathematical modeling

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Chapter 1

General Introduction

1.1 Population growths and consequences

The world population is anticipated to increase by 21% by 2040 [1]. Due to this population growth, the energy demand rises consequently. Figure 1 shows the projected worldwide rise in energy consumption from 1980 to 2030. Also, fossil fuel consumption in a period of 20 years (from 2000 to 2020) has shown a rise of 32% [2], [3]. Fossil fuels such as coal, oil, and natural gas have been the dominant energy sources over the last few years, and they cover up to 95% of the energy demand in the world [2], [4]. Burning fossil fuels release CO_2 gases, contributing to more than 78% of the total increase in greenhouse gas (GHG) emissions from 1970 to 2010 [5]–[7]. CO_2 emissions are the primary reason for climate change [8].

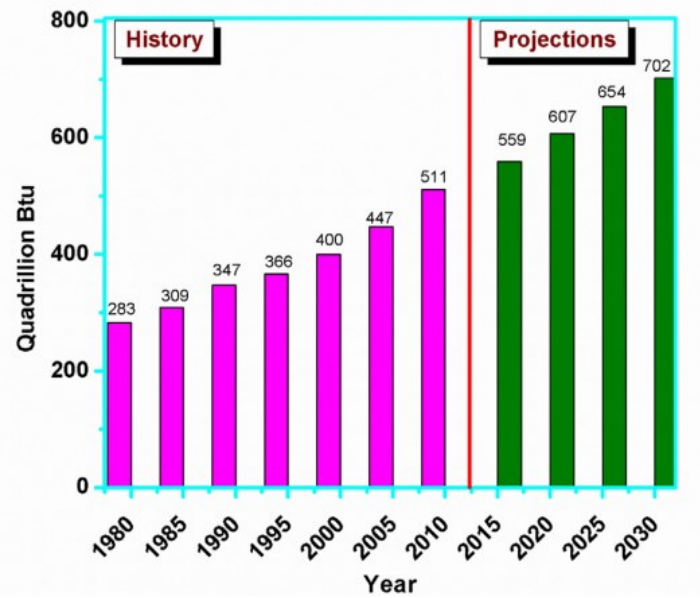


Figure 1. A review of global energy consumption over a period of 50 years [2].

1.2 Clean and sustainable energy sources

Looking for new energy sources without any harmful impacts on the environment and long-lasting energy supply to address energy demand growth is vital [2]. To ensure a sustainable and clean future, studies on finding alternative renewable and green energy resources to replace conventional fuels such as heavy fuel oil, combat climate changes, and reduce greenhouse gas emissions are

increasing exponentially [9], [10]. In recent years, many countries have put their effort into using renewable energy resources, including solar, hydrogen, ocean thermal energy, biomass, geothermal, tidal, biogas, biofuel, hydropower, and wind power, instead of fossil fuels [2], [11]. An overview of population growth and environmental impacts are shown in Figure 2.

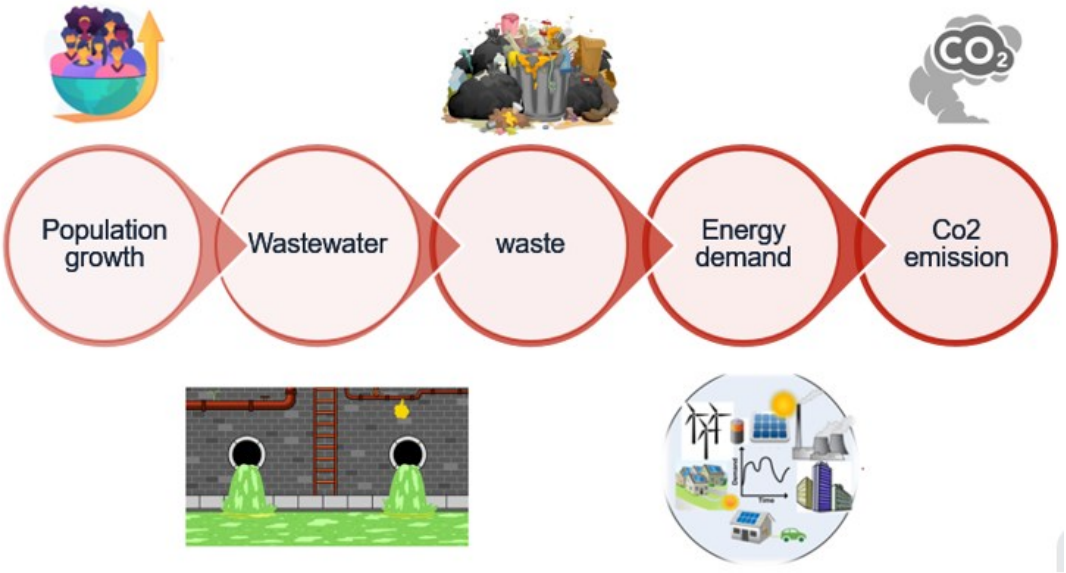


Figure 2. Population growth and environmental impacts.

1.3 Hydrogen as a clean and renewable source of energy

During the last few years, researchers focused on hydrogen to establish an environmental-friendly and reliable alternative fuel and energy storage option [12]. Hydrogen is known as the lightest, most abundant, and emission-free fuel. The only by-product of burning hydrogen is water due to its clean-burning qualities [2]. Hydrogen as an alternate fuel has high energy density, and low volumetric energy density. Energy derived from 1 kg of hydrogen is equal to energy extraction from 1 gallon of gasoline [2], [13]. Some characteristics of hydrogen are shown in Table 1.

Table 1. The thermos-physical characteristics of hydrogen [20]–[22].

Characteristics	Value (ref)	Characteristics	Value (ref)
Auto-ignition temperature	400-585 ℃	Lower heating value (LHV)	120 MJ/kg at 298 K
Octane number	>130	Higher heating value (HHV)	141.8 MJ/kg at 298 K
Value of solid, liquid, and Gas (at 1 bar and 20 ℃)	1kg, 14,104 L and 12,126 m3	Flash point	-253℃
Flammability range %	4-75	Critical temperature, Pressure, and density	-239.9 ℃, 1296.212 kPa, and 30.12 kg/m^3
Flame temperature	1526.85℃	Specific heat at constant pressure and volume	14.34 kJ/(kg ℃), 10.12 kJ/(kg ℃)

Hydrogen storage, distribution, and production from renewable and sustainable resources such as water electrolysis (WE) running by a wind turbine or solar panels do not pose any pollution risks [14], [15]. The types of hydrogen are classified as green, blue, and grey based on production pathways and raw material sources [10]. Hydrogen production via fossil fuels such as SMR (steam methane reforming) produces carbon emissions, and it is known as grey hydrogen. But if there are any carbon capture facilities to store or reuse the exhausted CO_2 for other applications, it is called blue hydrogen [10], [16]. Green hydrogen is produced from renewable energy sources, and there are no emissions or environmental issues during their production process [17], [18]. Some kinds of technologies for grey, blue and green hydrogen production are categorized in Table 2.

Table 2. Grey, blue, and green hydrogen production methods [2], [27].

Type of hydrogen	Source of energy or feed	Methods
Grey	Fossil-based energy sources (natural gas, oil, coal)	Autothermal reforming (ATR) Steam methane reforming (SMR) Chemical looping reforming (CLR)
Emission condition	Without a carbon capture system	

Blue	Fossil-based energy sources (natural gas, oil, coal)	Autothermal reforming (ATR) Steam methane reforming (SMR) Chemical looping reforming (CLR)
Emission condition	With carbon capture systems	
Green	the endless energy source such as : (solar, wind, biomass, water, wastewater, solid waste, sewage sludge)	-Water electrolysis -Biological hydrogen production (Fermentation, bio-photolysis, microbial electrolysis cell, microbial fuel cell, Bio-catalyzed electrolysis) -Pyrolysis -Biomass-gasification -Thermochemical water splitting -photocatalytic decomposition of water
Emission condition	Carbon emission-free	

1.4 Wastewater and water scarcity

Large amounts of wastewater production and water scarcity are other global issues due to population growth. Today, there is more pressure on water supply and sewer systems due to urbanization, and the energy use by these sectors is much higher than before [19], [20]. It is predicted that freshwater availability may decrease by 40% in the next decades [21]. Additionally, large amounts of wastewater from different sectors, such as industrial, domestic, and agriculture, are collected and transferred daily to wastewater treatment plants (WWTPs). According to statistics, approximately 10^9 cubic meters of urban wastewater are produced annually worldwide [12], [22]. Some kinds of wastewater treatment pathways are listed below [23]–[25]:

- Conventional aerobic activated sludge treatment
- Anaerobic digester
- Membrane technology
- Ion exchange
- Adsorption
- Chemical precipitation
- Coagulation
- Electrolytic reduction

- Flocculation
- Froth flotation

Each of the technologies above has its own drawback. These may include high energy demand, cost-intensive, large residual generation, ineffective in utilizing the energy potential from wastewater, complexity, and not being environmentally friendly [26], [27]. Thus sustainable techniques for green energy extraction from wastewater and treatment simultaneously are gaining much interest among scientists.

Carbon chains are one of the main contents of wastewater, and it should be noted that any compound containing carbon is known as an organic matter, and they are viable energy sources [28], [29]. As wastewater is rich in organic matter, it can be considered a renewable resource for energy production [21], [30]. For instance, it is estimated that every liter of domestic wastewater contains 7.6 kJ energy [31]. To make use of this energy content, Bio-electrochemical systems (BESs) can be applied for wastewater treatment and generate hydrogen or electricity.

1.5 Bio-electrochemical systems (BESs)

Bio-electrochemical systems (BESs) can use waste material for energy generation [2]. BESs combine biological and electrochemical methods to convert the bio-waste to electricity or chemicals [32], [33]. They can be used for simultaneous waste or wastewater treatment and energy generation [34], [35]. Biological processes are catalyzed by microorganisms that exist in bio-waste under atmospheric pressure and ambient temperature [36], [37]. The raw material for BES processes is well-accessible. Moreover, there is no need to transport the waste or wastewater to any location for the purpose of treatment by applying these technologies locally [2]. In BESs, biological processes, enzymes, or microorganisms are utilized to generate electricity or other valuable products [38]. BESs consist of anodic and cathodic compartments [33]. Basically, the cathodic compartments are considered an electrode for the acceptance of oxygen [39]. Also, to prevent oxygen penetration into the anode chamber, an ion-exchange membrane is supposed to separate the two compartments in cells [40]. During the BESs cell chemical processes, acetates or formates are produced because biocatalysts biologically break down the carbon substrate in solutions [33]. In addition, the growth of biofilms on the surface of the electrodes [41] and direct electron transfer occur at this time to reach the main goal for electricity or chemical energy production [33].

1.6 Components of BES cells

1.6.1 Electrodes

Cathode and anode are two solid electric conductors that carry the electric current in BESs. The performance of BESs depends on the electrode material. The material selection for electrodes is affected by many factors such as excellent conductivity, enhanced mass transfer, large surface area, low price, mechanical strength, scalability, biocompatibility, and chemical stability. Carbon felt carbon mesh, graphite fiber brush, and carbon cloth are appropriate for anode fabrication [42]. Furthermore, platinum and graphite are proper materials to create the cathode electrode [33]. Platinum is the best option for the oxygen reduction reaction. Also, in MECs, platinum is one of the best catalysts for hydrogen evolution reactions [43].

1.6.2 Membrane

There are two types of membranes in BESs, including penetrable and non-penetrable membranes. The penetrable membranes employ charge and neutral transfer between two chambers, but non-penetrable membranes are applied for both charge transfer and prevent the oxygen crossover to the other side [44]. Also, it is important to know that sometimes there is no need to use ion-exchange membranes [45].

1.6.3 Substrate

The substrate's nature, constituents, and concentration affect the microbial community and the energy recovery, including power or hydrogen generation during the cell operation. For instance, glucose, cellulose, sodium acetate, oil refinery waste, agro-process waste residuals, and dairy and vegetable waste are feedstock in BESs. They give energy to bacterial cell development [46]–[48].In most cases, acetate is considered a main substrate because its energy is higher than that of other substrates [46].

1.6.4 Transfer of Electrons

Only a few microbes are capable of the current generation, and the efficiency of the BESs depends on the rate of movement or transport of electrons to the sides of the electrode via available microorganisms in wastewater flows or sewage sludge [49]–[53]. The transfer of electrons in bio-electrochemical systems occurs via a direct or indirect process (see Figure 3). Our focus in our research is based on indirect electron transfer, which is explained as follows [54] :

- ❖ Mediators are electrochemical active groups responsible for redox and oxidation reactions.
- ❖ Indirect electron transfer occurs via mediators shuttled between microorganisms and substrates instead of bacteria to the anode surface area.
- ❖ They equally affect the interaction between the cell and the surface of the electrodes.

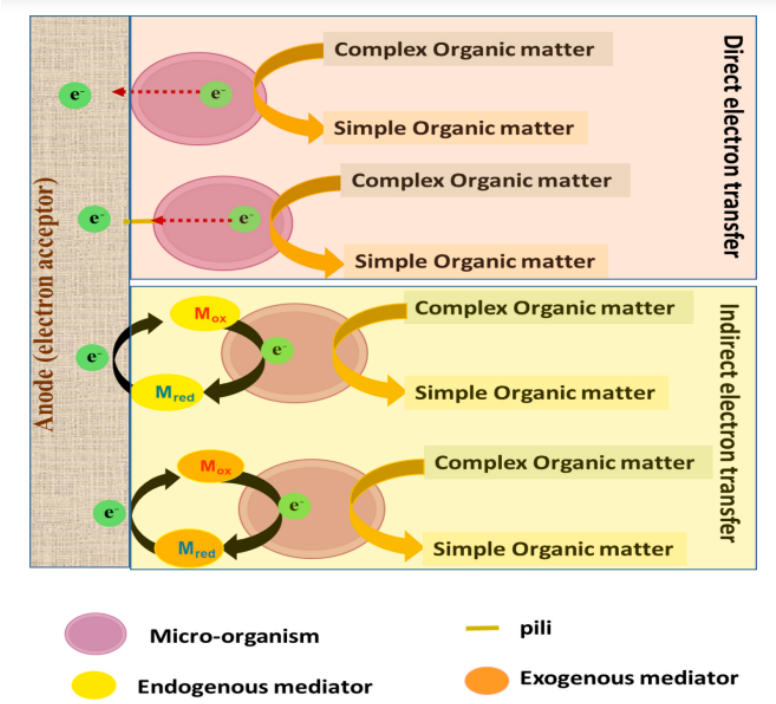


Figure 3. The schematic of direct and indirect electron transfer in bio-electrochemical systems [33].

Some kinds of BESs are listed below [55] :

- Microbial electrolysis cells (MECs)
- Microbial fuel cells (MFCs)
- Microbial desalination cells (MDCs)
- Enzymatic biofuel cells (EBCs)
- Microbial reverse electro-dialysis cells (MRECs)
- Microbial solar cells (MSCs)
- Microbial electro-synthesis cells (MESCs)

1.7 Introduction to Microbial electrolysis cells (MECs) and Microbial fuel cells (MFCs)

Among different types of BESs, MECs and MFCs are novel technologies that use microorganisms to transform wastewater into hydrogen and electricity, respectively, as their main product. Energy in the form of electricity and hydrogen can be extracted from wastewater during treatment, providing products that can help offset treatment costs. MFC has been examined as a method for generating electricity while simultaneously treating wastewater. In these systems, bacteria oxidize organic matter and release electrons to an anode, which then go through the cathode and combine with oxygen and protons to form water. MEC is a new and promising technology that can convert soluble organic matter of wastewater into storable chemical energy, such as hydrogen. So, Hydrogen gas can be generated from biomass using electro-hydrogenizes in a microbial electrolysis cell. The MEC is a modified MFC in which the cathode is completely anoxic, and an external voltage is added to produce hydrogen by using the bacteria.

The University of the West of England, Wetsus and Wageningen University, and the University of Science & Technology of China carried out the first investigation on electricity generation with the aid of MFCs [56]–[58]. Also, researchers have studied MECs for the production of hydrogen and ammonium recovery in the last decades [59]. A general view of MEC and MFC is demonstrated in Figure 4.

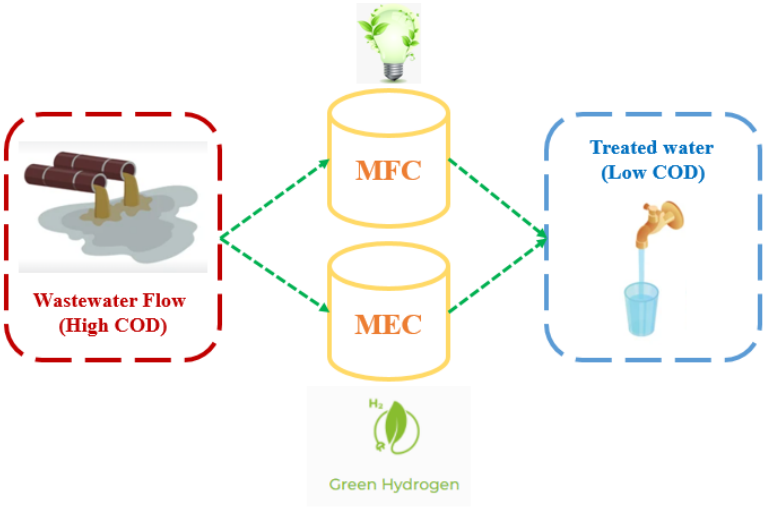


Figure 4. A general view of MFC and MEC.

1.8 The advantages of using MEC and MFC as wastewater treatment techniques

The growth in freshwater demand and wastewater generation leads to more pressure on wastewater and water treatment plants, especially in urban areas [60], [61]. Modern Wastewater treatment methods that treat wastewater in the same location of production alleviate the necessity of piping and sewer systems to collect the wastewater for treatment plants and decrease the amount of freshwater from the sources. Moreover, applying MECs and MFCs as an urban wastewater treatment infrastructure has the potential to reduce the cost of wastewater treatment and sludge disposal and accumulation [62]. Then treated wastewater can be used for various applications such as toilet flushing, irrigation, cleaning, car-washing, and laundry as a consequence of treating wastewater locally. On top of that, MFCs and MECs are remarkable wastewater treatment pathways over the typical technologies due to microbial metabolic activities for energy production without high energy input and less carbon emission [63], [64]. They consume waste material as input for green hydrogen and electricity generation. To put it another way, they treat waste material as well as clean and renewable energy production [65].

In terms of hydrogen production, the studies have shown that the bio hydrogen production yield via MECs is about 40%-70% more than dark fermentation [65]. Also, the main advantage of MECs versus WE for hydrogen generation is that the oxidation of water is replaced by the oxidation of organic compounds, which can occur at significantly lower redox potentials and lower input voltage required [66].

1.9 Research objectives:

The need for clean energy and cost-effective low-energy wastewater treatment becomes greater day by day. Additionally, the rise in greenhouse gases and climate change puts more pressure on governments to dedicate more budget to advance technologies for green energy production. Around 20% of total global energy demand is related to the residential sectors in the form of heating, cooling, and lighting the residential dwellings [67]. In addition, people living or working in residential or commercial buildings generate wastewater daily. By applying MFCs and MECs in buildings, wastewater could be treated and reused in different applications such as toilet flushing, car-washing, and irrigation. The produced hydrogen via MEC can be stored and converted in fuel cells to generate the electricity necessary for lighting, heating, and cooling systems, or it can be used as a transportation fuel. Hence, working on new and advanced

technologies which treat wastewater and generate power simultaneously can improve the energy efficiency of buildings. Moreover, it should be noted that compost is a by-product of this process, which could be used for rooftop gardens. This process has some bottlenecks that restrict the upper boundary of hydrogen yield. Further, MFC and MEC technologies are still in their infancy, facing unresolved challenges that need to be addressed in order to scale up the technology for commercialization. Therefore effective parameters should be found and optimized in this process. Thus in this study, the potential of applying new technologies, including MFCs and MECs for wastewater treatment and energy recovery, will be investigated. The large-scale usage of the mentioned advanced technologies needs to be modeled in the first step.

In this regard, the research objectives for this study are as follows:

- Develop a mathematical model of SCMEC and DCMEC.
- Comparison between SCMEC and DCMEC outputs concerning hydrogen production.
- Estimation of electricity generation via fuel cells by using the generated hydrogen from MECs.
- Mathematical modeling of dual-chamber MFC.
- Comparison between electricity generation via MFCs and MECs-FC (both types).
- Define two scenarios and case studies based on real data to examine the feasibility of using MECs and MFCs for residential and commercial buildings in urban areas.
- Comparisons between BESs and WWTPs regarding electricity consumption.
- Hydrogen production comparisons via MECs and water electrolyzers.
- Assess the potential usage of the generated power and hydrogen via BESs in transportation sectors.

Chapter 2

Microbial Fuel Cell & Microbial Electrolysis Cell

MFCs and MECs are made up of anode and cathode electrodes, substrates, ion exchange membranes, and microbial communities [33]. The energy in terms of electricity or hydrogen can be obtained via microbial reactions and charge transfers occurring at the anode and cathodic compartments. The substrate breakdown using active bacteria occurs at the anode chamber, and electrons and protons release in this area. Then only protons are permitted to pass through the ion-selective membrane from the anode side to the cathode side, and electrons flow to the cathode chamber via an external circuit. For both chambers, chemical reactions take place in the absence of oxygen (anaerobic conditions) in MECs. But, for power generation, the cathode chamber in MFCs needs to run the reactions in the presence of oxygen (aerobic conditions) [68]. It should be noted that both MEC and MFC release carbon dioxide based on their chemical reactions [33]. The factors that affected both MFCs and MECs' performance are shown in Figure 5.

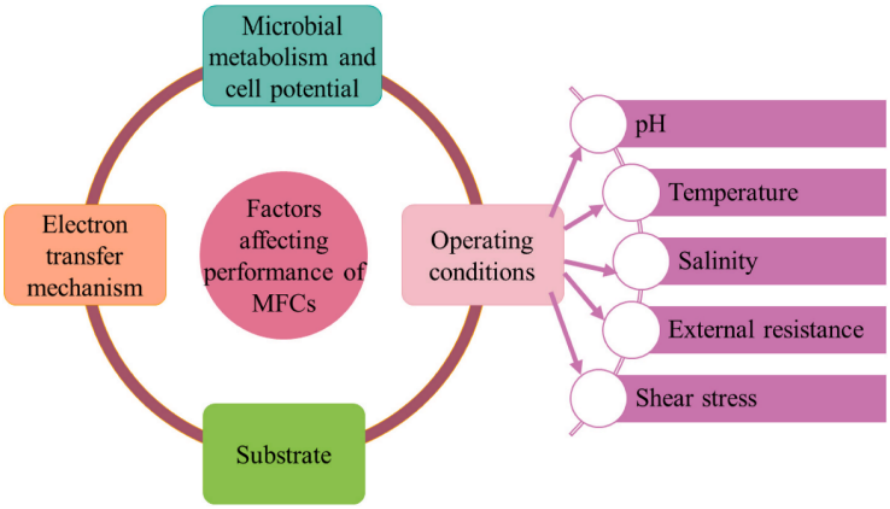


Figure 5. The factors affecting MFCs and MECs performance **[27]**.

2.1 Microbial fuel cell (MFC):

One of the most common types of BESs are MFCs that utilize domestic or industrial wastewater to convert chemical energy into electrical energy and treat wastewater simultaneously [27]. Microbes in MFCs are able to extract electrical energy from the breakdown of organic matters that exist in wastewater flows [69]. Up to 4 to 15 W power density per cubic meter of industrial or domestic wastewater can be generated via MFCs from industrial and domestic wastewater [70]–

[72]. Two-chamber MFCs are more typical and common than a single chamber one, and in most of the studies, a two-chamber MFC is assumed for examinations. In a two-chamber MFCs, bacteria in the anode chamber are separated from the cathode chamber by a polymeric proton exchange membrane. Figure 6 shows a schematic of a typical dual chamber MFC. Then Figure 7 shows some types of MFCs configuration, and their descriptions are categorized in Table 3

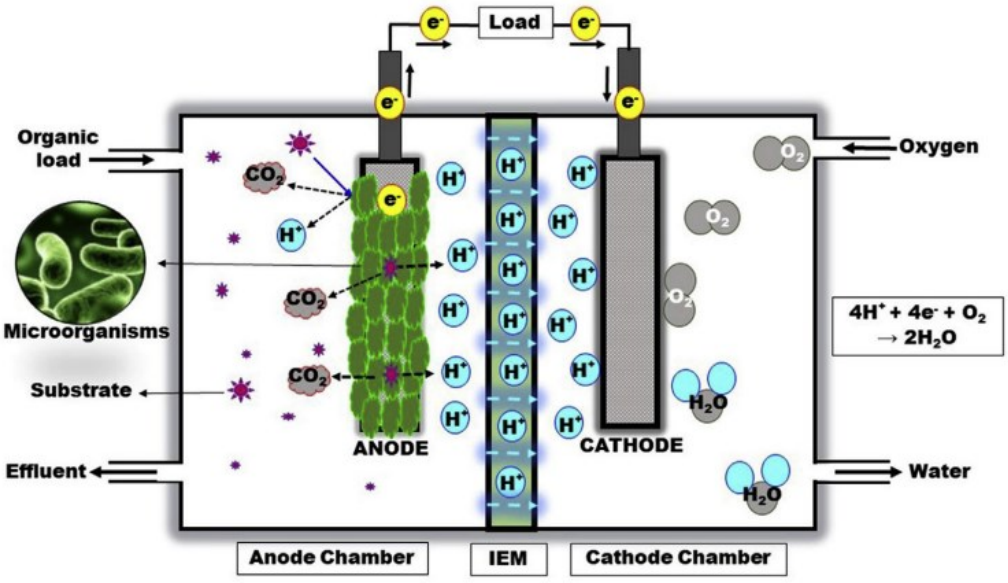


Figure 6. Schematic of typical dual chamber MFC **[26]**.

Also, the chemical reactions in MFCs are listed below:

Anode compartment reactions:

$$C_2H_4O_2 + M_o \rightarrow M_r + CO_2 \quad (1)$$

$$M_r \rightarrow M_o + e^- + H^+ \quad (2)$$

$$C_2H_4O_2 \rightarrow CH_4 + CO_2 \quad (3)$$

Cathode compartment reaction:

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

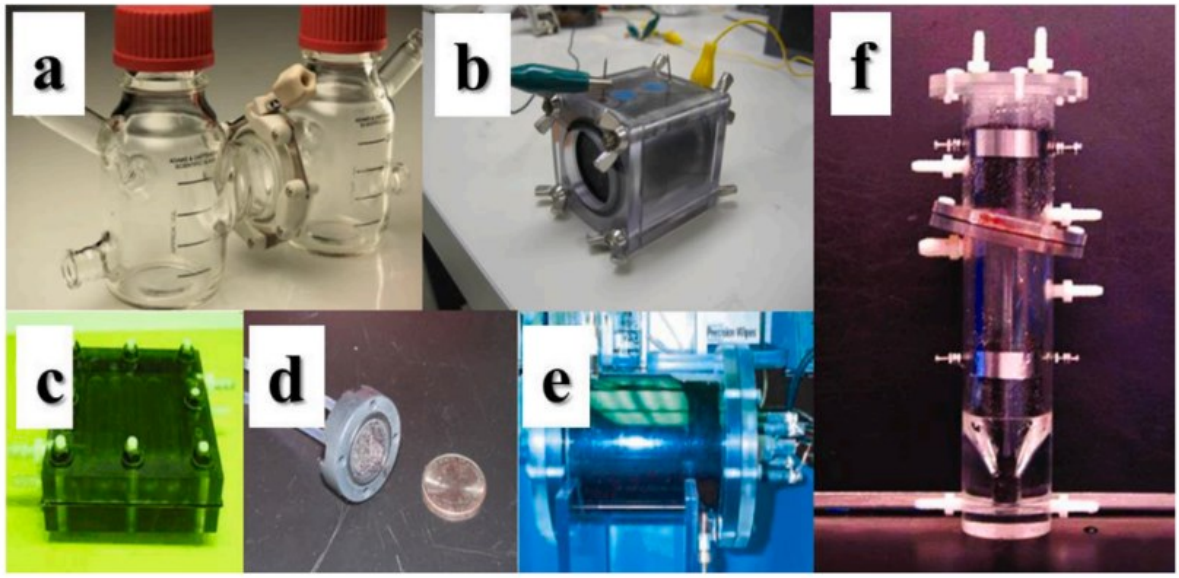


Figure 7. Different configurations of MFC **[27]**.

Table 3. Description of different configurations of MFC.

Alphabet	Type of MFC	Special specification	Ref.
a	H-type	Inexpensive platform and generate a low power density that can be attributed to lower membrane surface areas for proton transfer	[27], [73]
b	Cube-type	Higher power density than H-type by maximizing the membrane surface	[27], [74], [75]
c	Flat-plate		
d	Miniature	have been developed for long-term, self-sustaining operation in large-scale power generation systems	[27], [76]
e	Horizontal tubular	The best option the examine different parameters for scale-up of MFCs for maximum power generation and wastewater treatment	[27], [77], [78]
f	Vertical tubular		

2.2 MFCs literature review

2.2.1 Experimental section:

For the first time, Liu et al. [79] demonstrated that domestic wastewater could be used as the substrate in single-chamber MFCs for power generation without feeding air into a cathode chamber. Brewery wastewater was examined by Feng et al. [72] in 2007. Their results show that decreasing the temperature will reduce the maximum power density and buffering capacity and strongly affect reactor performance. For instance, the cell's power output will be increased by adding more phosphate buffer. In addition, Liu and Logan.[70] used domestic wastewater in a two-chamber MFC to assess power generation in an air-cathode MFC enclosing carbon electrodes in the presence and absence of a (PEM). They replaced the aqueous cathode with the previous one, and the results have shown an increase in generated power. Moreover, they have investigated the effect of the presence and absence of proton exchange membrane (PEM). Their final outputs reveals that the absence of PEM leads to more power generation due to a higher cathode potential.

2.2.2 Modeling section:

The research community has worked on different MFC models such as electrochemical, biochemical, and transport phenomena equations, electron transfer mechanism, fluid dynamics, operational parameters, catalyst redox activities, and physical characteristics [79]–[81]. MFCs need to be modeled with engineering perspectives in terms of optimum operating conditions to get higher performance and energy recovery for scaling up applications. Some modeling approaches have been proposed for the MFC system in recent years. Pinto et al. [82] took a two microbial population MFC modeled to compare different operating modes and reactor configurations. The results indicated that the electrical load could control the ratio between the anodophilic and methanogenic populations, and the co-existence of the two populations reduced reactor performance. They concluded that if reactors were connected in series, they would certainly improve treatment efficiency. The authors improved their previous study by applying ordinary differential equations to calculate real-time process control to define biomass growth and retention in the anode chamber [83]. They found that the highest generated electricity of MFC was achieved by changing the operating conditions, which made the proposed model suitable for a convenient tool for off-line process optimization.

Oliveira et al. [84] executed a one-dimensional model for MFC, and they monitored the system's performance by changing the current density that affected over-potential loss; they noticed that changing substrate concentration and operating temperature influenced biofilm thickness as well. The simulated model was appropriate for generating the required power for real applications, improving MFC understanding, and optimizing fuel cell design and operation. Karamzadeh et al. [85] conducted a sensitivity analysis of MFC to investigate the impact of the start-up method, feed concentration, and anode electrode surface area on the performance of MFC. They found that enhancing the external resistance, COD, and anode surface area led to increased power generation. Esfandyari et al. [86] considered a model based on an artificial neural network (ANN) and adaptive neuro-fuzzy inference system (ANFIS) to investigate the effect of power density and columbic efficiency (CE) in an MFC. Ionic strength, initial pH, medium nitrogen concentration, and temperature have been selected as operation variables. Their investigation indicated that for predicting power density and CE of MFC based on the ionic strength, initial pH, medium nitrogen concentration, and temperature, the ANN and ANFIS models had acceptable performance. On the other hand, ANN model had a more straightforward structure and tuning procedure than the ANFIS model.

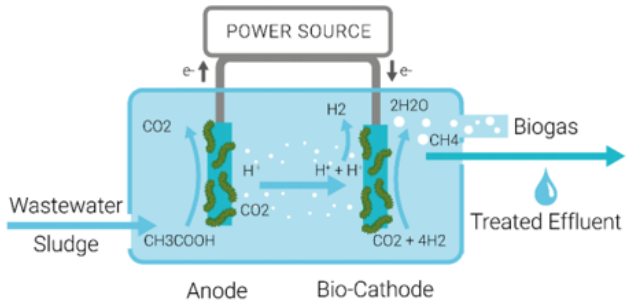
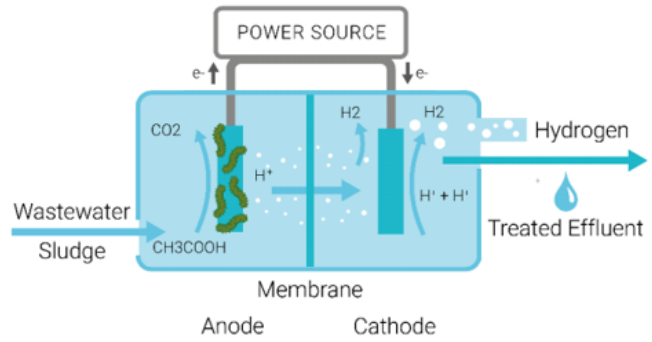
2.3 Microbial electrochemical cell (MEC)

MECs were introduced in 2005 as a promising and well-investigated type of BESs, except that it involves a sealed cathode and external voltage to generate bio-hydrogen [87], [88]. MECs utilize organic matter as a source of electrons via microbes to produce bio-hydrogen and treat the waste flows [89], [90]. In an anode chamber, active microorganisms electrochemically use organic matter to generate protons, CO_2, and electrons [91]. Most of the energy comes from the chemical energy extracted from substrates oxidized at the anode side [92]. Then generated electrons are transferred to the cathode side through an external circuit to combine with protons to generate hydrogen in the absence of oxygen [93]. This approach is more efficient than WE since the external voltage needed for hydrogen production in MECs is much less than in conventional ones. Some of the strengths (S) and weaknesses (W) of hydrogen production via MECs are listed in Table 4.

Table 4. The strengths (S) and weaknesses (W) of hydrogen production via MECs.	
References: [9], [33], [94]–[97]	
(S). Process conditions for hydrogen production in MECs are simple. They only need acetates as a substrate and 0.11 V applied voltage.	(W). The commercialization of the MECs for large-scale production is the main weakness or barrier of this viable technology. Some of these e factors that were responsible for mentioned challenges are listed below: The reactor geometry Electrode material Glass fiber separators Possible connection resistances Microbiological factors lead to slow start-up for the reactor
(S). The external energy needed in MECs is less than WE for hydrogen production, which is around 4.5-5.0 kW h/m^3. Also, this value for hydrogen production via MECs is about 1-3 kW h/m^3.	
(S). Compared with other hydrogen production methods, the purity of hydrogen production via MECs is higher.	
(S). The generated hydrogen through MECs is free of sulfur, and it is ideal for various applications.	(W). The external energy sources are needed to operate MECs.
(S). MECs can be integrated with different existing technologies in terms of advanced industrial applications.	(S). MECs are sustainable options for decentralized wastewater treatment and hydrogen production.

In aspects of configuration, there are two types of MECs, single and dual chambers. A membrane separates MECs cathode and anode chamber in the dual chamber. However, single chamber MECs can reduce the cost of construction and operation, but it has a drawback regarding the activity of hydrogenotrophic microorganisms that use generated hydrogen and CO_2 to form the extra methane and decrease the purity of hydrogen gas in outputs [62]. Therefore, in most recent studies, dual-chamber configurations are considered in all pilot-scale research to test the potential of using MECs as a conventional system for wastewater treatment. All chemical reactions related to the SCMEC and DCMEC accompanied by their schematics are demonstrated in the below table.

Table 5. The chemical reactions and schematics of single and dual chamber MECs [108].

Type of MECs	Chemical Reaction
Single Chamber (MEC_S) 	Anode compartment reactions: $C_2H_4O_2 + 2H_2O + 4M_o \rightarrow 4M_r + 2CO_2$ (5) $4M_r \rightarrow 4M_o + 8e^- + 8H^+$ (6) $CO_2 + HCO_3^- + 8e^- + 8H^+ \rightarrow CH_3COO^-$ (7) Cathode compartment reaction: $C_2H_4O_2 \rightarrow 4CH_4 + CO_2$ (8) $CO_2 + 4H_2 \rightarrow CH_4 + 2H_2$ (9) $2H_2O + 2e^- \rightarrow 2OH^- + H_2$ (10)
Dual Chamber (MEC_D) 	Anode compartment reactions: $C_2H_4O_2 + 2H_2O + 4M_o \rightarrow 4M_r + 2CO_2$ (11) $4M_r \rightarrow 4M_o + 8e^- + 8H^+$ (12) $C_2H_4O_2 \rightarrow CH_4 + CO_2$ (13) Cathode compartment reaction: $2H_2O + 2e^- \rightarrow 2OH^- + H_2$ (14)

The chemical reaction in MECs is not thermodynamically favorable, and an external energy source is needed to drive the reduction reaction to produced hydrogen via these technologies [98]. Also, the required external energy can be optimized by considering a lower pH on the cathode side, which enhances the potential of the cathode compartment. But, an electrolyte pH value of less than 5 causes a restriction on the migration of protons via the membrane, and they return to the anode side [33]. Therefore, lower pH at the anode compartment has detrimental impacts on microorganism activities.

2.3.1 Power sources for MECs:

The price of the input electricity for hydrogen production from renewables and green technologies such as WE is the main challenge in addition to high capital cost [10], [99]. They are usually integrated with renewable energy sources like wind turbines or solar panels to provide the required energy for their operations see figure 8. Among different types of renewable energy resources, the power from solar panels and wind turbines is the most abundant and environmentally friendly [100]. Hence, by harvesting solar and wind energy, green hydrogen can be generated through MECs [101].

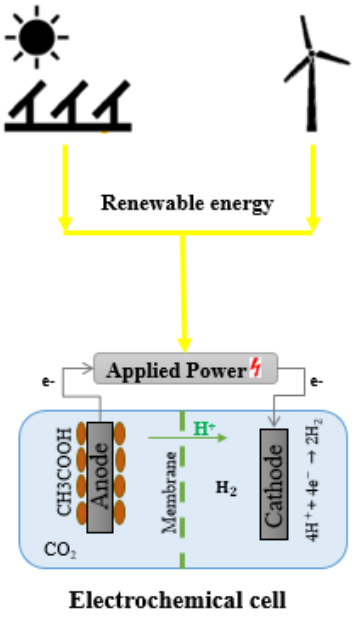


Figure 8.The integration of solar panels and wind turbines with BESs.

2.4 MECs literature review

There has been a rise in research areas relating to microbial electrolysis cells for hydrogen production from organic waste during the last decades. There is a lot of research on different aspects, such as mathematical modeling and laboratory tests, but there are still some barriers prior to commercializing MECs. It needs to be optimized in several critical features, such as maximizing the hydrogen production, using lower-cost energy input, and cost of the construction and total process [33], [98]. Various developments and improvements concerning cell design [102]–[104], removal membrane [105]–[108], utilization of microbial catalysts [109], and increase in hydrogen

production [110]–[112] have been determined, but, it still needs more effort to make it a viable process for using in industries and large scale H_2 production [113], [114]. Besides hydrogen, other valuable chemicals such as methane, acetate, hydrogen peroxide, ethanol, and formic acid could be produced via MECs [114]–[116].

2.4.1 Experimental section:

A few pilot scales of MECs for domestic and urban wastewater treatment have been investigated over the last few decades. Some of the experimental lab-scale and pilot-scale of MEC are listed in Table 6. They focused on main objectives such as organic load, applied voltage, temperature, inoculum, and pH to obtain higher yields of hydrogen production. Also, the EcoVolt reactor from the Cambrian company was the first commercial application of MEC in the United States. An anaerobic treatment solution eliminates BOD and generates renewable biogas from high-strength wastewater streams, producing clean water and clean energy. EcoVolt is ideal for facilities generating wastewater flows between 4,000 and 1,250,000 gallons per day [117].

Table 6. MEC experimental studies.

Parameters	Cusick RD et al. [118]	Gil-Carrera L et al. [119]	Heidrich et al. [120]	Heidrich et al. [97]	S. E. Cotterill et al. [121]	Baeza JA et al. [122]
Type of influent	Domestic Wastewater	Urban Wastewater	Domestic Wastewater	Domestic Wastewater	Urban Wastewater	Urban Wastewater
Type of Reactor	SC	SC	DC	DC	DC	DC
Reactor volume (L)	0.028	10	120	120	175	130
Operation Mode	B*	C*	C*	C*	C*	C*
HRT (h)*	24	10	21	24	5	48
Applied voltage (v)	0.9	0.9	1.1	1.1	0.9	1.5
Gas production rate (m^3H_2/m^3. d)	0.028	0.05	0.015	0.007	0.005	0.032
H_2 Purity (%)	70	-	100	98-99	93	94
Coulombic efficiency (%)	64±5	23	55	41	43	28
COD Removal (%)	58±3	76	34	65.6	63.5	25
Temperature (°C)	31	23-25	13.5-21	1-22	11.4±2.5	18-22

HRT: Hydraulic Retention Time, SC: Single Chamber, DC: Dual Chamber

2.4.2 Modeling section:

Besides experimental studies, mathematical modeling is necessary to find the best approaches regarding the best operational conditions physical, chemical, and biological processes involved in the bioreactors and optimize them for increasing hydrogen production rate and efficient wastewater treatment. Therefore, a few studies have been conducted recently in the aspect of modeling.

In 2011 two research studies were done by Pinto et al.[123], [124] to analyze hydrogen production via MECs. The first one presented a unified dynamic model for both MEC and MFC to generate hydrogen and electricity, respectively, and the only difference in their equation was related to the cathode side. For process control approaches, their results could be applied. The second one was optimized hydrogen and electricity generation via MEC and MFC by selecting optimal operating current. The results showed that the current could determine the proportion of the different microbial populations in anodic biofilm. Moreover, in 2012 Pinto et al. [125] proposed a multi-population dynamic model of a MEC at continuous operation fed with acetate or synthetic wastewater. Their model was conducted based on the microbial growth of some microorganisms, which demonstrated the influence of applied voltage and organic load on hydrogen production. They reached a good agreement with the experimental data, which resulted in maximizing hydrogen production and achieving the desired level of COD removal simultaneously under-considered operational parameters. Also, internal resistance had a considerable effect on optimal operating current. Karla M et al. [126] developed a 3D model for MEC to investigate distributions of current, potential, and concentrations and their effect on potential distribution over the surface of electrodes to evaluate the reactor performance. The results revealed that flow pattern and electric field influenced reactor behaviors and experimental data of external current and hydrogen generation versus time in feeding cycles were close to the model results of integrated current density over electrode surfaces. Sewsynker et al. [127] used five artificial neural networks to model complex and non-linear processes for hydrogen generation via MECs. Substrate type, concentration, PH, temperature, applied voltage, and reactor configuration were their model inputs that played a crucial role in MECs performance. Also, they used 50 data points to predict their results, indicating a strong validation of observed data. The proposed model could be used to the optimized window in MEC scale-up processes. Alavijeh et al. [79] proposed a model for both MECs and MFCs. At first, they modeled MFC based on experimental results and various simulated

variables of liquid bulk and biofilm. Secondly, they extracted the MEC model from MFC by changing boundary conditions. So, as an innovation, they introduced biofilm local potential modeling for MEC simulation with simple linear boundary conditions. Therefore, the performance of MEC was identified according to the variations of microbial distributions, methane, and hydrogen production at different applied voltage. In addition, they simulated polarization characteristics reached from experimental data. All these valuations specified that the proposed model was successfully able to predict both MFC and MEC performance.

Luis Blanco-Cocom et al. [128] presented a mathematical model of stirred fermenter connected to a bio-catalyzed electrolysis cell for continuous hydrogen production. According to partial data and unknown initial conditions, the model could estimate parameters in ordinary differential equations by using a hybrid of a genetic algorithm and least squares. The proposed model expressed the dynamics of hydrogen and volatile fatty acid production and substrate consumption. Also, a hybrid evolutionary algorithm and squares method was used to estimate the parameters. Yahya et al. [129] modified an existing MEC model based on a multi-population model based on material balance with the integration of bio-electrochemical reactions describing the steady-state behavior of biomass growth, consumption of substrates, and hydrogen production, and the effect of applied voltage on the performance of the MEC. The model was analyzed and tested with open-loop simulation results to obtain the maximum hydrogen production rate and the current from wastewater in a fed-batch reactor. Also, hydrogen production was optimized by selecting the optimal current and applying a voltage to the MEC. Mardanpour et al. [130] were the pioneer in proving the ability of MEC as a promising technology in medical applications due to the following factors: significant bio-hydrogen generation, low consumption of expensive materials, simple construction, and utilization of human excreta. By conducting an experimental study, they concluded that amongst electrodes, nickel caused the highest performance to generate hydrogen. Also, they applied a modeling approach based on chemotaxis phenomena which resulted in having the best configurations since they could be compatible with real conditions. Their model had good behavior at higher voltage because of attaching bacteria and improving the extracellular polymer substance content of the biofilm. A dynamical model for MEC_D was proposed by Estrella et al. [131], which was derived from the mass balances of a continuous flow system. It was described by three ordinary differential equations (ODEs), which let a fast convergence without the numerical solution of non-linear algebraic equations. They compared two microbial populations

and proved that their concentration had a substantial impact on hydrogen and methane production rates, especially during the initial stages of the MEC. The proposed model was suitable for off-line process optimization and real-time process control. The authors performed steady-state analysis and concluded that only one of the three possible steady states was stable. Gonzalez et al. [132] simulated a continuous MEC model with Matlab based on the behavior of substrate consumption, microbial growth, competition between anodophilic and methanogenic microorganisms for the carbon source in the anode, hydrogen generation, and electrical current production. In the modeling, dilution rate and applied potential were selected as two control approaches. Based on the modeling results, both control laws could respond adequately and efficiently to the disturbances and reach the reference value they were subjected to. The authors used control inputs including applied potential and dilution rate to increase the generation of hydrogen and indicated that the former and later were feasible for a short and long period of time respectively.

2.5 Hydrogen as a main product of MECs

The main valuable product of MECs is hydrogen. Hydrogen has a wide range of applications, and it could be used in a diversity of sectors such as turbines, internal combustion engines, fuel cells, kitchen ovens, and heaters. Also, it could be added to other fuels to form enriched energy mixtures [133]. In addition, when it comes to mobility triggers, hydrogen as a green fuel for powering electric vehicles via batteries or fuel cells would be highlighted [134]. It is predicted that in the United States, by the year 2050, the demand for hydrogen will reach around 42 million metric tons per year, which can fuel up 342 million light-duty vehicles for 51×10^{11} miles of travel per year [133].

Chapter 3

Methodology and Mathematical Modeling

3.1 Introduction to mathematical modeling

This chapter contains mathematical modeling of three types of continuous flow bio-electrochemical reactors, including:

I. Single Chamber Microbial Electrolysis Cell (SCMEC)
II. Dual Chamber Microbial Electrolysis Cell (DCMEC)
III. Microbial Fuel cell (MFC)

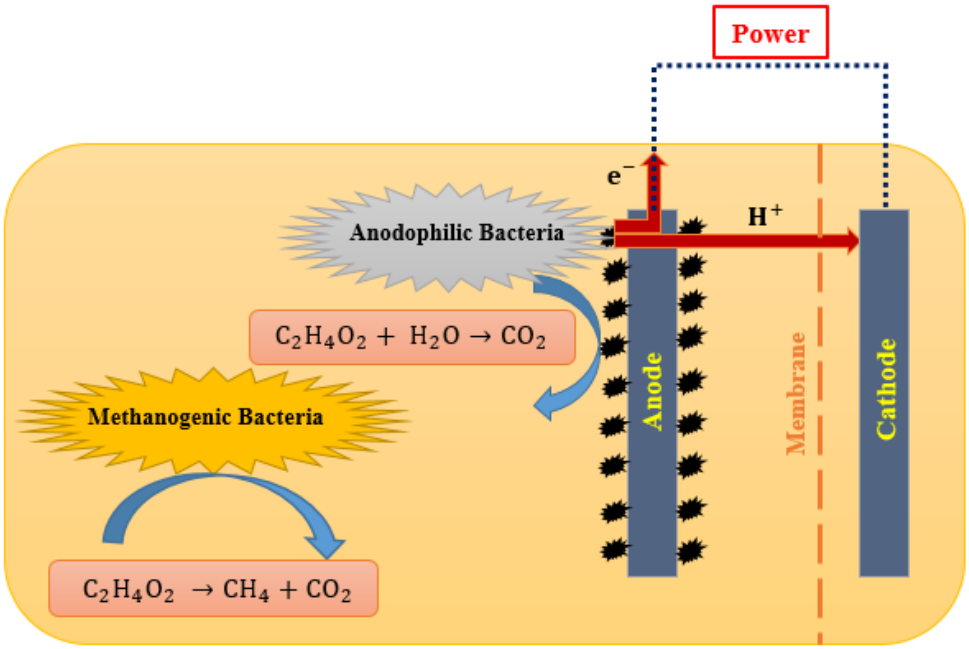
All have been considered for wastewater treatment and energy recovery.

In this research, the mathematical modeling of proposed bio-electrochemical systems is based on competition between microbial populations, including anodophilic and methanogenic, for the consumption of the main carbon source in the anode chamber. Besides anodophilic and methanogenic, hydrogenotrophic microorganisms exist in SCMEC. Acetate is considered the main carbon source in this study, and 550 mg/l is the assumed soluble amount of acetate in wastewater. In the first step, the model is developed for a 1-liter reactor volume, and then it is examined for two case studies on a large scale.

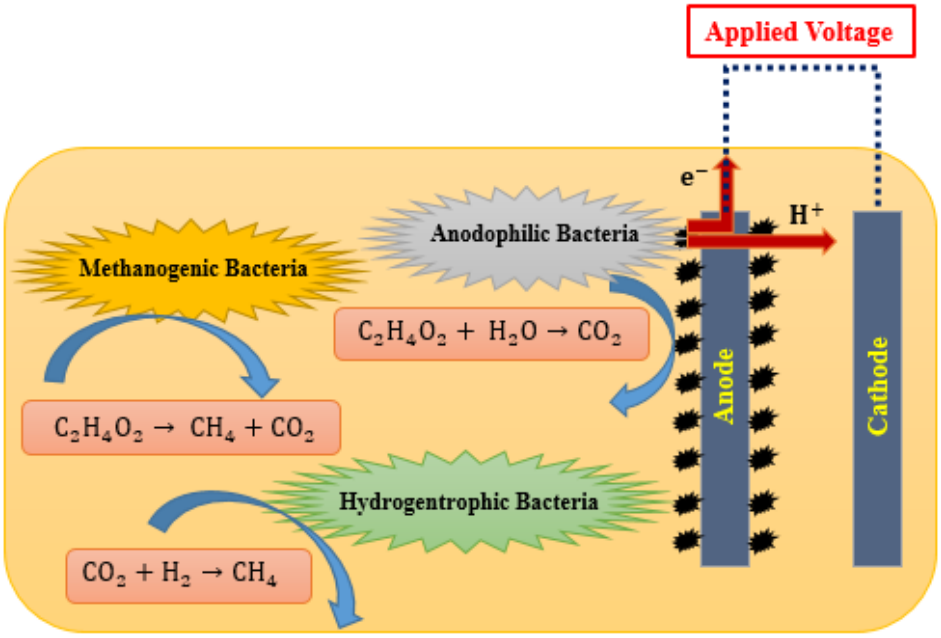
Figure 9 demonstrates the view of interactions between microorganisms and substrates in assumed solutions. It is shown that in both MFC and DCMEC, the anodophilic and methanogenic bacteria are active in consuming acetate. The anodophilic bacteria release electrons and protons plus CO_2, but the product of consumption of acetate with methanogenic are methane and CO_2. So the desired microorganism is anodophilic because of the releasing the charge. There is a significant difference in the SCMEC. One more microorganism comes into the picture, which is known as hydrogenotrophic bacteria. The role of these microorganisms is to mix the CO_2 and H_2 to form methane. The mass balance equations describe the behavior of substrate consumption, microbial growths, and competition, and a fast numerical solution is needed to solve the differential equations related to biomass growth and retention in the anodic compartment.

Moreover, in respect of the charge transferring mechanism from a carbon source and anodophilic microorganisms to the anode, as explained in chapter 1, the charge is assumed to involve intracellular mediators, which exist in the reduced and oxidized forms.

A. Microbial Fuel Cell



B. Single Chamber (MEC)



C. **Dual Chamber (MFC)**

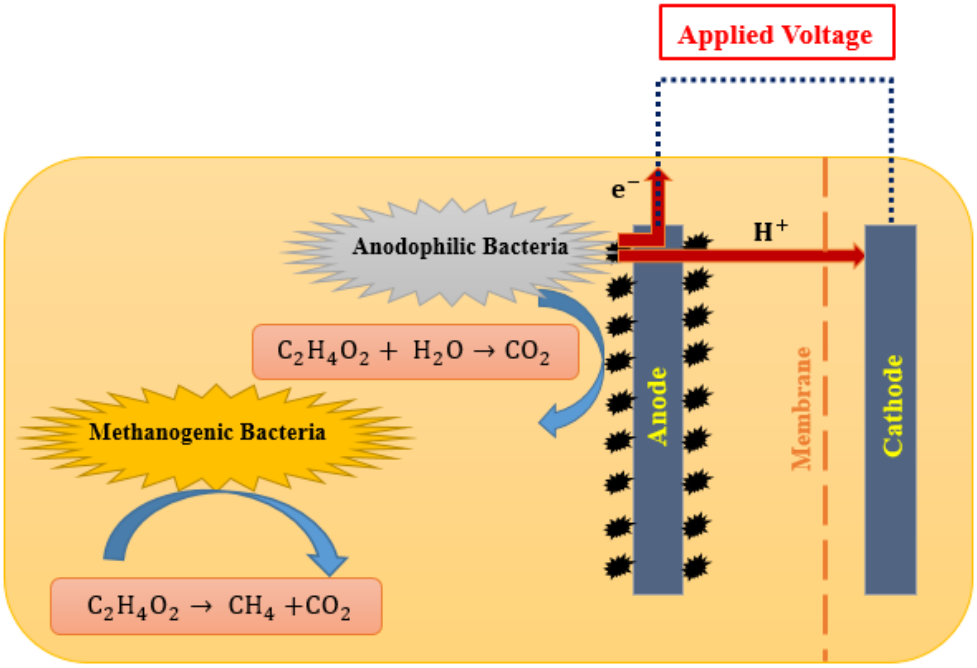


Figure 9. The distribution of microbial populations in the anode chamber (A, B, C).

In the following, all equations needed for the dynamical modeling of mentioned technologies are exhibited in different sections. Also, in previous studies, researchers used ODE15 as their numerical solving method for ordinary differential equations (ODEs), but in this study, Radau approaches have been used for the first time, which is more described in the following sections. Model validation and results for two case studies are published in the next chapter.

3.2 Assumptions for mathematical modeling

Some of the modeling assumptions which are common in all three technologies are listed below:

I. Essential indicators, including pH, temperature, and pressure, are constant during the chemical processes in MEC and MFC.
II. Microbial population and bio-electrochemical reaction are considered only in the anode chamber.
III. The uniform distribution of microbial populations and ideal mixing is assumed in the anode part.
IV. In exist bio-electrochemical systems (BES), where substrate gradient in the biofilm is neglected.
V. The non-limiting cathode reaction rate is assumed.
VI. Acetic acid is considered the primary substrate (carbon source) in this study(S).
VII. M_o , M_r are the concentration of oxidized and reduced forms of intracellular mediator, respectively. They are responsible for charge transfer from anodophilic bacteria to the electrode surface area in the anode chamber.
VIII. External circuits are in charge of electron transfer between the anode and cathode chamber as an extracellular electron transfer.
IX. Anodophilic bacteria are only attached to the electrode, but methanogenic are in both types of attached or suspended to the electrode (see Figure 9).
X. Dilution rate (D parameter) is estimated according to the below equation

$$D = \frac{F_{inlet}}{V_r}$$

Where F_{inlet} is the input flow.

3.3 Constant values for mathematical modeling of both MEC and MFC

For each mathematical model, some constant values and variables are needed during the modeling processing. Hence, the constant values are brought together in Table 7.and the other parameters will be mentioned in continue for each technology separately.

Table 7. Universal Constant values for Model MEC and MFC ([137], [138]).					
F	Faraday constant	96485 (C/mol)	R_1	Ideal constant of gases	8.314 (J/mol.K)
F_1	Faraday constant	1.1167 (A.d/mol)	m	Electrons per mol of mediator	2 (mol e^-/mol H_2)
R	The ideal constant of gases	0.08205(L.atm/mol.K)	H_2	Saturation of H_2 in water	1 (mg A /L)
T	Temperature	298.15 K	P	Pressure	1 atm
F_{inlet}	Inlet flow	1 liter/day	V_r	Reactor volume	1 liter

3.4 Mathematical Modeling of SCMEC and DCMEC

The proposed model for SCMEC and DCMEC in this study has been adapted from some researches [123], [125], [129], [131], [132]. The presented model is developed based on competition between three microbial populations, including anodophilic and methanogenic acetoclastic bacteria as a sole acetic acid consumers. Hydrogentrophic bacteria use mineralized carbon (CO_2) and hydrogen to produce methane. Table 8 reveals all mathematical equations for modeling two configurations of MEC containing both SCMEC (S) and DCMEC (D).

Table 8. Equations for Modeling of SCMEC (S) & DCMEC (D) [17], [108], [135], [137], [138].

Categories	Type of equations	Type of MEC
Mass balance equations		
(S) Main substrate (mg_S/L)	$\frac{dS}{dt} = \frac{F_{inlet}}{V_r}(S_0 - S) - q_a X_a - q_m X_m$ (15)	S,D
(X_a)Anodophilic microorganism (mg_X/L).	$\frac{dX_a}{dt} = \mu_a X_a - K_{d,a} X_a - \alpha_1 \frac{F_{inlet}}{V_r} X_a$ (16)	S,D
(X_m)Acetoclastic methanogenic microorganism (mg_X/L).	$\frac{dX_m}{dt} = \mu_m X_m - K_{d,m} X_m - \alpha_1 \frac{F_{inlet}}{V_r} X_m$ (17)	S,D

(X_h)Methanogenic hydrogenotrophic microorganism (mg_X/L).	$\frac{dX_h}{dt} = \mu_h X_h - K_{d,h} X_h - \alpha_2 \frac{F_{inlet}}{V_r} X_h$ (18)	S
Note : α_1, α_2 (biofilm retention)		
Hydrogen production rate equations		
Hydrogen (L_{H2} /d)	$Q_{H_2} = Y_{H_2} \frac{I_{MEC}}{mF_1} \frac{RT}{P} - Y_h \mu_h X_h V_r$ (19)	S
Hydrogen (L_{H2} /d)	$Q_{H_2} = Y_{H_2} \frac{I_{MEC}}{mF_1} \frac{RT}{P}$ (20)	D
Note: Hydrogen consumption by anodophilic microorganisms in an anode chamber is neglected.		
Intracellular mass balances equations		
Intracellular mediator (mg_M/mg_X)	$M_{total=} M_r + M_o$ (21) $\frac{dM_o}{dt} = \frac{\gamma}{V_r X_a} \frac{I_{MEC}}{mF_1} - Y_M q_a$ (22)	S,D
Microbial Kinetic equations		
Growth rate(1/d)	$\mu_a = \mu_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_{MEC} + M_o}$ (23)	S,D
	$\mu_m = \mu_{max,m} \frac{S}{K_{s,m} + S}$ (24)	S,D
	$\mu_h = \mu_{max,h} \frac{[H_2]}{K_h + [H_2]}$ (25)	S
Note: μ_a,μ_m,μ_h are the growth rate of anodophilic microorganism, acetoclastic methanogenic microorganisms, and Methanogenic hydrogentrophic microorganisms, respectively.		
Substrate consumption rates by microbial population (mg_S/mg_X d)	$q_a = q_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_{MEC} + M_o}$ (26)	S,D
	$q_m = q_{max,a} \frac{S}{K_{s,m} + S}$ (27)	S,D
Note: q_a , q_m are anodophilic microorganisms and acetoclastic methanogenic substrate consumption.		
Electrochemical equations		
electrochemical equilibrium	$E_{app} = E_{CEF} - \eta_{ohm} - \eta_{conc} - \eta_{act}$ (28)	
Ohmic resistance	$\eta_{ohm} = R_{int} I_{MEC}$ (29)	
Losses	$\eta_{conc} = \frac{R_1 T_{MEC}}{mF} \ln(\frac{M_T}{M_r})$ (30)	

	Note: η_{Conc} is the concentration losses and the concentration losses at the cathode is neglected.	S,D
	$\eta_{act} = \frac{R_1 T}{\beta m F} \sinh^{-1}(\frac{I_{MEC}}{S_A i_0})$ (31) Note: η_{act} is an activation losses.	
Current density generated by anodophilic microorganisms	$I_{MEC} = \frac{E_{CEF} + E_{app} - R_1 T[\ln(\frac{M_T}{M_r}) + \frac{1}{\beta}\sinh^{-1}(\frac{I_{MEC}}{S_A i_0})]}{R_{int}}$ (32) Note: It is assumed that $\varepsilon \approx 0$	
	$R_{int} = R_{MIN} + (R_{MAX} - R_{MIN})e^{-k_R X_a}$ (33)	
Current density generated by anodophilic microorganisms	$E_{app} = E_{CEF} - \eta_{ohm} - \eta_{conc} - \eta_{act}$ (34)	

The biofilm formation is divided into two layers, and homogeneous distribution of microorganisms for each layer is assumed [135]. Each layer is not able to hold more than a maximum attainable biomass concentration (X_{max}). Also, stationary phase and steady state thickness are assumed for biofilm approaches [136].The first layer stands for anodophilic and the second one stands for acetoclastic methanogenic microorganisms, respectively. The biofilm retention constant for both SCMEC and DCMEC is based on equation 35 [124].

α_1 : If $X_a + X_m \geq X_{max,1}$ then

$$\alpha_1 = \frac{(\mu_a - K_{d,a})X_a + (\mu_m - K_{d,m})X_m}{X_a + X_m} \quad (35)$$

Otherwise $\alpha_1 = 0$

α_2 : If $X_h \geq X_{max,2}$ then $\alpha_2 = \mu_h - K_{d,h}$

Otherwise $\alpha_2 = 0$

3.4.1 Design parameters (SCMEC & DCMEC)

The model parameters are extracted from the literature and are listed in the table below.

Table 9. Design parameters (MEC) ([137], [138]).

Γ	Mediator molar mass	663400 (mg M/mol M)	R^*_{min}	Lowest internal resistance observed at start-up conditions	2 (Ω)
E_{app}	Applied potential	0.6 (V)	R_{max}	Highest internal resistance observed at start-up conditions	200 (Ω)
E_{CEF}	Counter electromotive force for the MEC	-0.35 (V)	β	Oxidation transfer coefficient or reduction	0.5
$[H_2]$	Dissolved hydrogen saturated concentration	1.5 (mg/L)	S_A	The surface area of the anode	0.01 (m2)
i_0	Exchange current density under reference conditions	1 (A/m2)	$X_{max,1}$	Maximum achievable biomass concentration for layer 1	512.5 (mg X/ L)
K_h	Half–rate constant for hydrogenotrophic microorganisms	0.001 (mg/L)	$X^*_{max,2}$	Maximum achievable biomass concentration for layer 2	1215 (mg X /L)
K_R	Constant, which determines the slope of the curve in the equation	0.024 (L/ mg X)	$\mu_{max,a}$	The maximum specific growth rate for anodophilic microorganisms	1.97 (1/d)
$K_{d,a}$	The decomposition rate of anodophilic microorganisms	0.04 (1/d)	$\mu_{max,h}$	The maximum specific growth rate for hydrogenotrophic microorganisms	0.5 (1/d)
$K_{d,h}$	The decomposition rate of	0.01 (1/d)	$\mu_{max,m}$	The maximum specific growth rate	0.3 (1/d)

	hydrogenotrophic microorganisms			for methanogenic microorganisms	
$K_{d,m}$	The decomposition rate of methanogenic microorganisms	0.01 (1/d)	M_T	Total of mediating fraction	1000 (mg M /mg X)
$K_{S,a}$	Half–rate (Monod) constant for anodophilic microorganisms	20 (mg S/L)	Y_h	The yield rate for hydrogen consuming methanogenic microorganisms	0.05 (ml H_2/ mg X)
$K_{S,m}$	Half–rate (Monod) constant for methanogenic microorganisms	80 (mg S/L)	Y_{H_2}	Hydrogen yield	0.9
K_{MEC}	Half–rate constant for the oxidized intracellular mediator	0.01 (mg M/L)	Y_M	The yield rate for the oxidized mediator	3.3 (mg M/mol A)
$q_{max,a}$	Maximum anodophilic reaction rate	13.14 (mg S/mg X d)	α_1	Dimensionless biofilm retention constant (Anodophilic microorganism, Layer 1)	0.5410
$q_{max,m}$	The maximum methanogenic reaction rate	14.12 (mg S/mg X d)	α_2	Dimensionless biofilm retention constant (Acetoclastic methanogenic microorganism, Layer 2)	0.4894

3.4.2 Initial value of (SCMEC & DCMEC)

For solving the ODE equations below, initial values have been adapted see Table 10.

Table 10. The Initial value of (MECs) ([137], [138]).		
M_{o_0}	Iv concentrations of oxidized intracellular mediator	100 mg M/ mg X
X_{a0}	Iv anodophilic microbial population	400 mg/L
X_{h0}	Iv methanogenic hydrogenotrophic microbial population	10 mg/L
X_{m0}	Iv acetoclastic methanogenic microbial population	50 mg/L
S_0	Iv Main substrate	1500 mg/L
I_{MEC_0}	Iv current density	0.001 A

Iv: Initial value

3.5 Mathematical Modeling of MFC:

The mathematical model for power generation through MFC has been considered for the co-existence of methanogenic and anodophilic microbial populations [83]. The following equations can describe the conceptual MFC model see 11.

Table 11. Equations for Modeling of MFC [93].

Type of equations	Variables	Equations
Mass Balance	(S) Main substrate (mg_S/L).	$\frac{dS}{dt} = D(S_0 - S) - q_a X_a - q_m X_m$ (36)
	(X_a)Anodophilic microorganism (mg_X/L).	$\frac{dX_a}{dt} = \mu_a X_a - K_{d,a} X_a - \alpha_a D X_a$ (37)
	(X_m)Acetoclastic methanogenic microorganism (mg_X/L).	$\frac{dX_m}{dt} = \mu_m X_m - K_{d,m} X_m - \alpha_m D X_m$ (38)
Production Rate	Methane (L_{CH_4}/d)	$Q_{CH_4} = Y_{CH_4} q_m X_m V_r$ (39)
		$M_{total=} M_r + M_o$ (40)

Intracellular mass balances	Intracellular mediator (mg_M/mg_X)	$\frac{dM_o}{dt} = -Yq_a + \gamma \frac{I_{MFC}}{mF} \frac{1}{V_r X_a}$	(41)
Microbial Kinetic	Growth rate(1/d)	$\mu_a = \mu_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_M + M_o}$	(42)
		$\mu_m = \mu_{max,m} \frac{S}{K_{s,m} + S}$	(43)
	Substrate consumption rates by microbial population (mg_S/mg_X d)	$q_a = q_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_M + M_o}$	(44)
		$q_m = q_{max,a} \frac{S}{K_{s,m} + S}$	(45)
Electrochemical		$I_{MFC} R_{ext} = E_{thermo} - I_{MFC} R_{int} - \eta_{conc} - \eta_{act}$	(46)
	Concentration losses	$\eta_{conc} = \frac{R_1 T}{mF} \ln(\frac{M_T}{M_r})$	(47)
	Activation losses	$\eta_{act} = \frac{I_{MFC}}{S_A i_{0.ref}} \frac{RT}{mF} (\frac{M_r}{M_o})$	(48)
	Current density generated by anodophilic microorganisms	$I_{MFC} = \frac{(E_{OCV} - \eta_{conc})}{(R_{Ext} + R_{Int})} \frac{M_r}{M_r + \varepsilon}$ It is assumed that ε ≈ 0.	(49)
	Internal resistance	$R_{int} = R_{MIN} + (R_{MAX} - R_{MIN}) e^{-k_R X_a}$	(50)
		$E_{ocv} = E_{Min} + (E_{Max} - E_{Min}) e^{\frac{-1}{k_R X_a}}$	(51)

OCV = Open circuit voltage

Calculation of biofilm retention constants for MFC:

In MFCs, there are two types of biofilm retention constant anodophilic (α_a) and acetoclastic methanogenic (α_m).They can be estimated by equation.52.

$$\alpha = \frac{1 + \tanh\left[K_x(X_a + X_m - X_{max})\right]}{2} \quad (52)$$

For calculation of these values, it is assumed that in the growth phase, no biofilm washout occurs so that a batch reactor balance can be used. During the static conditions, biofilm washout is considered equal to net biofilm growth. In other words, continuous stirred-tank reactor (CSTR) conditions are used for constant biofilm calculation on MFC.

3.5.1 Design parameters (MFC)

The model parameters are based on the available literature, which can be found in the following table.

Table 12. Design parameters (MFC) ([93], [137], [138]).

Parameter	Value and unit	Parameter	Value and unit
Y (mediator yield)	22.75 (mg M/mg S)	K_M(Mediator half-rate constant)	0.01 (mg M/L)
Y_{CH_4}(Methane yield)	0.3 (mL CH_4/ mg S)	$K_{d,a}$(Decay rate of anodophilic microorganisms)	0.04 (1/d)
$\mu_{max,a}$(Maximum anodophilic growth rate)	1.97 (1/d)	$K_{d,m}$(Decay rate of methanogenic microorganisms)	0.01 (1/d)
$\mu_{max,m}$(Maximum methanogenic growth rate)	0.1 (1/d)	$X_{max,a}$(Anodophilic biofilm space limitation)	512.5 (mg X/L)
$q_{max,a}$(Maximum anodophilic reaction rate)	8.48 (mg S /mg X d)	$X_{max,m}$(Methanogenic biofilm space limitation)	525 (mg X/L)
$q_{max,m}$(Maximum methanogenic reaction rate)	8.20 (mg S /mg X.d)	K_X(Steepness factor)	0.04 (L/mg X)
$K_{s,a}$(Half-rate constant of anodophilics)	20 (mg S/ L)	R_{max}(Maximum internal resistance)	2000 (Ω)
$K_{s,m}$(Half-rate constant of methanogens)	80 (mg S/ L)	R_{min}(Minimum internal resistance)	25 (Ω)
γ (Mediator molar mass)	663400 (mg M/$mole_{mediatore}$)	E_{Min}(Minimum E_{OCV})	0.38 (V)
M_T(Mediator fraction)	0.05 (mg M/ mg X)	E_{max}(Maximum E_{OCV})	0.66 (V)
K_R (Constant, which determines the slope of the curve in the equation)			0.006 (L/mg X)

3.5.2 Initial value of (MFC)

For solving the ODEs equation, some initial value is needed. Therefore the initial values applied to run the Radaue methods are indicated in Table 13.

Table 13. The initial value of (MFC) ([93], [137], [138]).		
M_{o_0}	Iv concentrations of oxidized intracellular mediator	0.2 mg M/ mg X
M_{r_0}	Iv concentrations of reduction intracellular mediator	0.8 mg M/ mg X
X_{a0}	Iv anodophilic microbial population	30 mg/L
X_{m0}	Iv acetoclastic methanogenic microbial population	50 mg/L
S_0	Iv Main substrate	600 mg/L
I_{MFC_0}	Iv current density	0.002 A

Iv: Initial value

3.6 Numerical methods and calculation

A dynamical mathematical model of single and dual chamber microbial electrolysis cell and microbial fuel cell has been implemented in Python. Fast numerical solutions of the model are assigned by using ordinary differential equations to describe biomass growth and retention in the anodic compartment.

Some stiff ordinary differential equations (Stiff ODEs) exist in the mass balance part and need to be solved using numerical solutions. In the numerical simulation of chemical processes, a significant task is integrating the stiff systems of ordinary differential equations describing the chemical transformations. In this regard, this study has solved Stiff ODEs by the fifth-order Radau method (IIA) [137]. Because Radau method has excellent stability properties when applied to stiff ODEs, it belongs to the class of fully implicit Runge–Kutta methods [138]. The below equations explain the Radau IIA method [139].

For the initial value problem, the below equations should be found:

$$y'(t) = f\big(t, y(t)\big), y(t)), y(t_0) = y_0$$
$$u_0 = y_0 \tag{53}$$

Then the $(i+1)^{th}$ iteration of a Runge-Kutta method with s stages is defined as:

$$u_{i+1} = u_i + h\sum_{j=1}^{s} b_j \,.\, f(t_i + c_j.h, u_{i+1}^{j}) \tag{54}$$

$$u_{i+1}^{j} = u_i + h\sum_{k=1}^{s} a_{jk}.f(t_i + c_k.h, u_{i+1}^{(k)}) \tag{55}$$

In the equation (42) and (43), the coefficients of c_1,c_2, c_3 …, c_s, and b_1,b_2, b_3, …, b_s, and a_{jk} are written as below:

$$\begin{array}{c|c} c_1 & \\ \vdots & \\ c_s & \end{array} \qquad \begin{bmatrix} a_{11} & \cdots & a_{1s} \\ \vdots & \ddots & \vdots \\ a_{s1} & \cdots & a_{ss} \end{bmatrix}$$

$$b_1 \quad \ldots \quad b_s$$

In this research, the stage of Radau IIA (s) is considered three, which resulted in having the order of five (2s-1). The stated order defines the weights of b_1,b_2, b_3,, c_1,c_2, c_3 that are adjusted into the first equations and the a_{jk} in to the second equation:

$b_1 = \frac{4}{9} - \frac{\sqrt{6}}{36}, b_2 = \frac{4}{9} + \frac{\sqrt{6}}{36}, b_3 = \frac{1}{9}, c_1 = \frac{2}{5} - \frac{\sqrt{6}}{10}, c_2 = \frac{2}{5} + \frac{\sqrt{6}}{10}, c_3 = 1$

Yields

$$u_{i+1} = u_i + h.\left(b_1.f\left(t_i + c_1h, u_{i+1}^{(1)}\right) + b_2.f\left(t_i + c_2h, u_{i+1}^{(2)}\right) + b_3.f\left(t_i + c_3h, u_{i+1}^{(3)}\right)\right) \tag{56}$$

$$u_{i+1} = u_i + h.\left(\left(\frac{4}{9} - \frac{\sqrt{6}}{36}\right).f\left(t_i + \left(\frac{2}{5} - \frac{\sqrt{6}}{10}\right)h, u_{i+1}^{(1)}\right) + \left(\frac{4}{9} + \frac{\sqrt{6}}{36}\right).f\left(t_i + \left(\frac{2}{5} + \frac{\sqrt{6}}{10}\right)h, u_{i+1}^{(2)}\right).f(t_i + 1h, u_{i+1}^{(3)})\right) \tag{57}$$

With

$$u_{i+1}^{(1)} = u_i + h.\left(a_{11}.f\left(t_i + c_1h, u_{i+1}^{(1)}\right) + a_{12}.f\left(t_i + c_2h, u_{i+1}^{(2)}\right) + a_{13}.f(t_i + c_3h, u_{i+1}^{(3)})\right) \tag{58}$$

$$u_{i+1}^{(2)} = u_i + h.\left(a_{21}.f\left(t_i + c_1h, u_{i+1}^{(1)}\right) + a_{22}.f\left(t_i + c_2h, u_{i+1}^{(2)}\right) + a_{23}.f(t_i + c_3h, u_{i+1}^{(3)})\right) \tag{59}$$

$$u_{i+1}^{(3)} = u_i + h.(a_{31}.f\left(t_i + c_1h, u_{i+1}^{(1)}\right) + a_{32}.f\left(t_i + c_2h, u_{i+1}^{(2)}\right) + a_{33}.f(t_i + c_3h, u_{i+1}^{(3)})) \quad (60)$$

The Radau IIA quadrature has the formula as:

$a_{11} = \frac{11}{45} - \frac{7\sqrt{6}}{360}$, $a_{12} = \frac{37}{225} - \frac{169\sqrt{6}}{1800}$,$a_{13} = -\frac{2}{225} + \frac{\sqrt{6}}{75}$, $a_{21} = \frac{37}{225} + \frac{169\sqrt{6}}{1800}$, $a_{22} = \frac{11}{45} + \frac{7\sqrt{6}}{360}$,

$a_{23} = -\frac{2}{225} + \frac{\sqrt{6}}{75}$, $a_{31} = \frac{4}{9} - \frac{\sqrt{6}}{36}$, $a_{32} = \frac{4}{9} + \frac{\sqrt{6}}{36}$, $a_{33} = \frac{1}{9}$

which can also be put in Butcher array as:

$$\begin{array}{c|ccc} \frac{2}{10} - \frac{\sqrt{6}}{10} & \frac{11}{45} - \frac{7\sqrt{6}}{360} & \frac{37}{225} - \frac{169\sqrt{6}}{1800} & -\frac{2}{225} + \frac{\sqrt{6}}{75} \\ \frac{2}{10} + \frac{\sqrt{6}}{10} & \frac{37}{225} + \frac{169\sqrt{6}}{1800} & \frac{11}{45} + \frac{7\sqrt{6}}{360} & -\frac{2}{225} - \frac{\sqrt{6}}{75} \\ 1 & \frac{4}{9} - \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{4}{9} - \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

By inserting the a_{jk} and $c_1, \ldots, c_3$ from the given butcher tableau, the new formula becomes:

$$y_{n+1} - y_n = h(\left(\frac{4}{9} + \frac{\sqrt{6}}{36}\right)k_1 + \left(\frac{4}{9} - \frac{\sqrt{6}}{36}\right)k_2 + (\frac{1}{9})k_3) \quad (61)$$

Chapter 4

Model Validation and results

4.1 Model validation

Model validation comes into the picture once the model development is finished. The most important part of model development processing is model validation. The fundamental role of model validation is the comparison of predictions from a current mathematical model of a system to the measured behavior of the systems in previous studies, including both experimental and computational model methodologies. On the whole, by successful model validation, the developed model is trustable and able to act robustly in future scenarios. In this section, microbial electrolysis cells and microbial fuel cells are validated by Gonzalez et al.[132] and R.P. Pinto et al.[83] works respectively. Also, in the following, the validation figures indicate the outputs of MECs and MFC models are well agreed with the previous modeling of other researchers. Moreover, in this study, the calculations of the mean squared error (MSE) formula are used to compare our model results with former research.

MSE formula :

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i^{Ref} - y_i^{sim}}{\bar{y}}\right)^2 \tag{62}$$

Where :

- N is the number of data points
- y_i^{exp} represented reference values
- y_i^{sim} represented simulation values

4.1.1 MEC model validation

In this simulation, the model outputs are validated by Gonzalez et al.[132] results. Figure 10, Figure 11, and Figure 12 depict the comparison between our model results and the work of Gonzalez et al. [132]. They show a good agreement between our simulation results and literature data. The simulation assessment regarding the generated hydrogen with those described by Gonzalez et al. [132] is shown in Figure 10. The hydrogen production rate rose significantly and reached nearly 8.5 l/day. Baucus, when the reactions start in bio-reactors, the accumulation of

organic matters and bacteria are at the highest level in the first five days. After that, in the rest of the process, it remains steady due to the continuous flow condition of operation. Also, the behavior of methanogenic (X_m) and hydrogenotrophic (X_h) microorganisms at the anode chamber of MEC during the chemical process is completely validated by Gonzalez et al. [132]. According to Figure 11 and Figure 12, at the beginning of the process, the population of methanogenic and hydrogenotrophic microorganisms is at the highest level, but they decrease over time to reach a value of zero. Because the methanogenic (X_m) consumes acetate to generate CO_2 and methane, and the hydrogenotrophic (X_h) use produced hydrogen and CO_2 to create methane which results in decreased hydrogen purity. However, the anodophilic microorganisms (X_a) compensate for the reduced amount of hydrogen by utilizing the main substrate and releasing protons and electrons. It leads to the growth of anodophilic population in the MEC and more hydrogen.

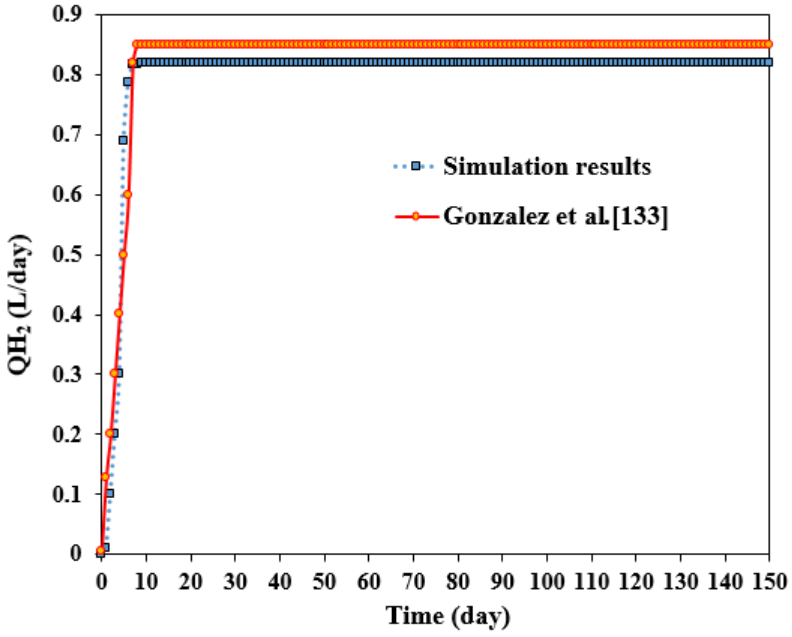


Figure 10. The hydrogen production rate (QH_2).

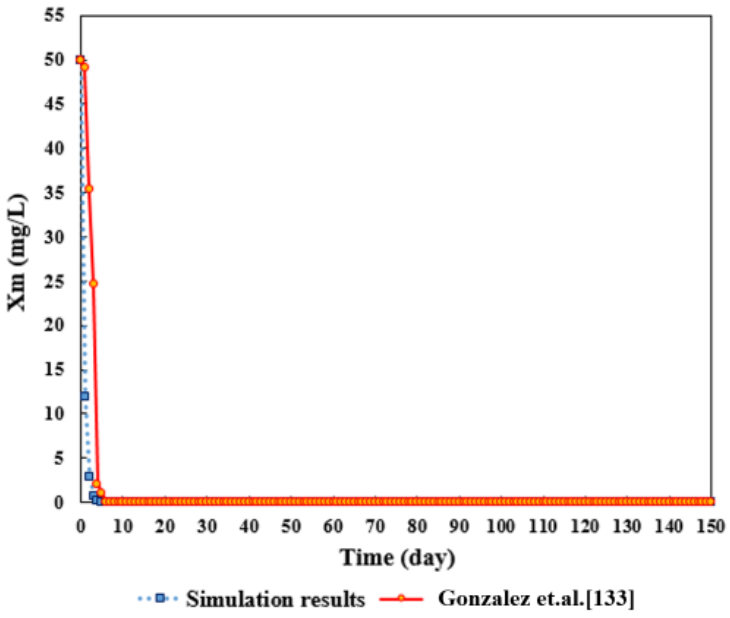


Figure 11. The behavior of methanogenic microorganisms (Xm).

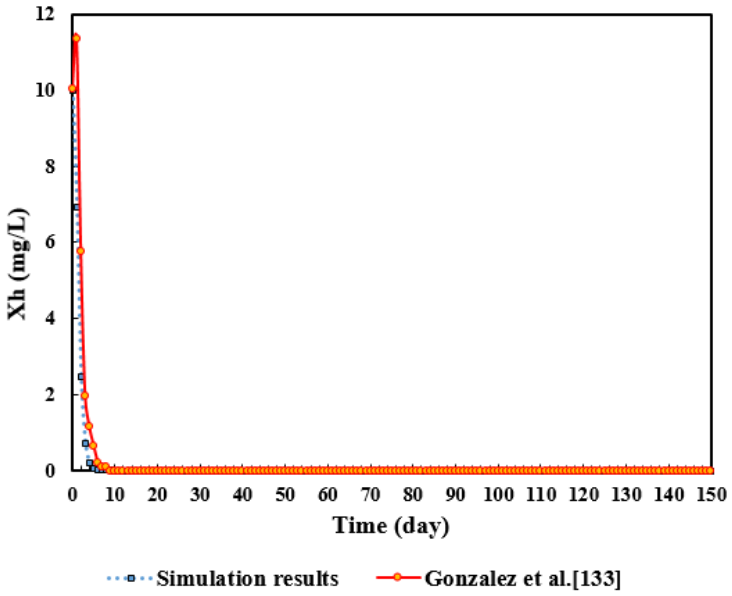


Figure 12. The behavior of hydrogenotrophic microorganisms (Xh).

In addition, calculations of the mean squared error (MSE) formula are used to compare our results with Gonzalez et al.[132] results in respect of hydrogen production rate, which is determined by 0.1%.

4.1.2 MFC model validation

To evaluate the MFC model accuracy, acetate consumption rate and methane production rate are compared with R.P. Pinto et al.[83] results. Figure 13, which is about the acetate concentration, shows that our model outputs are in good agreement with Pinto et al. [83]. It is demonstrated that the concentration of acetate at the beginning of the process is at the highest value, and during this time, it will be consumed by microorganisms. It goes to zero values with time. Figure 14 shows that the average daily methane outputs from our model could be about 0.67 (ml/liter of wastewater), closely following the reference measured.

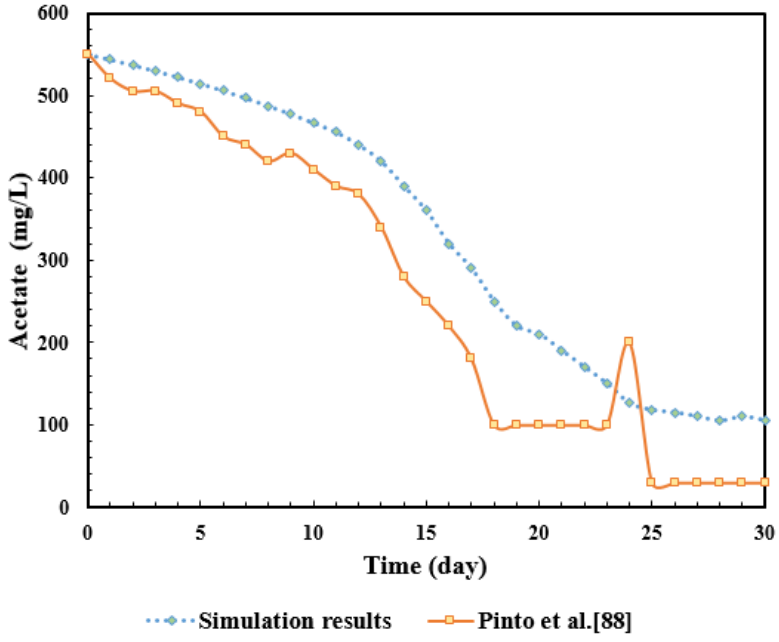


Figure 13. The acetate consumption rate.

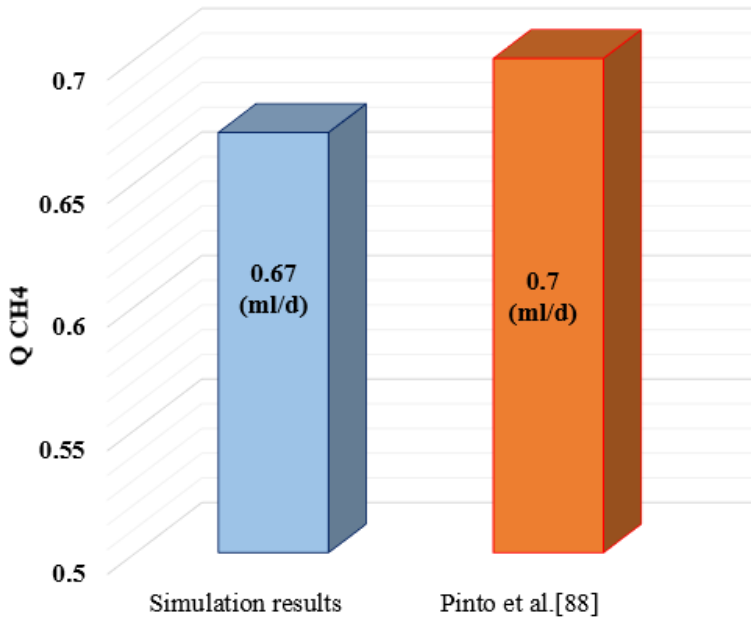


Figure 14. The average daily methane production per 1 liter of wastewater.

In addition, the mean squared error (MSE) formula is used to compare the results from the current model and Pinto outputs. In this regard, the calculation of MSE for acetate consumption and methane production is estimated at about 0.7 % and 0.09 %, respectively.

4.2 Model results

4.2.1 Results of the MEC models

In chapter three, both mathematical models of SCMEC and DCMEC were introduced. The hydrogenotrophic microorganism in the anode chamber is the only difference between these two kinds of models. The presence of hydrogenotrophic leads to two different hydrogen production rates, as appears below.

Table 14. Different hydrogen production rate equations in SCMEC and DCMEC.		
Hydrogen (L_{H2} /d)	$Q_{H_2} = Y_{H_2}\frac{I_{MEC}}{mF_1}\frac{RT}{P} - Y_h\mu_h X_h V_r$	SCMEC
Hydrogen (L_{H2} /d)	$Q_{H_2} = Y_{H_2}\frac{I_{MEC}}{mF_1}\frac{RT}{P}$	DCMEC

So, in the proposed model, the rate of hydrogen production in both SCMEC and DCMEC are compared see Figure 15. Since there is no membrane between the cathode and anode sides in the SCMEC, the produced hydrogen is consumed by hydrogenotrophic microorganisms, which leads to decreased hydrogen levels. The daily hydrogen production rate numbers are reported as about 0.52 L and 0.86 L for SCMEC and DCMEC per liter of wastewater, respectively. The membrane and cathode side in a dual-chamber helps the system have more hydrogen than a single one, as illustrated below.

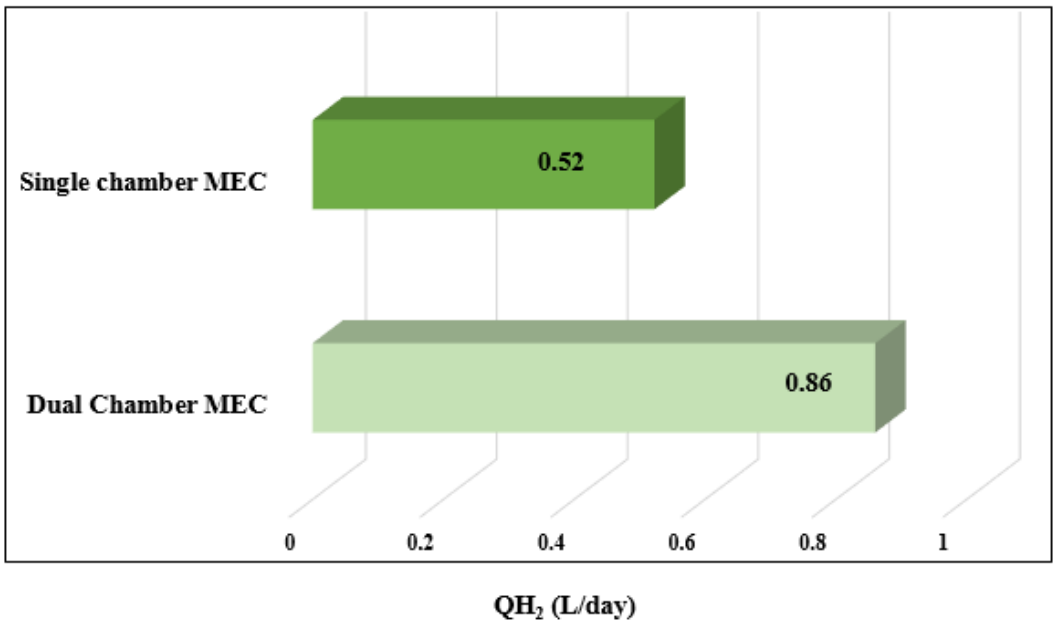


Figure 15. The daily hydrogen production rate is compared between single and dual chamber MECs per 1 liter of wastewater.

As methanogenic and hydrogenotrophic microorganisms consume acetate and hydrogen, they are known as undesired microbial populations. According to Figure 11 and Figure 12, hydrogenotrophic and methanogenic microorganisms reach zero value during the first five days, so it is expected to see a climb in the behavior of anodophilic and hydrogen production rates. In this regard, Figure 16 depicts growth in anodophilic microorganisms' behavior. It is concluded that growth in the population of anodophilic microorganisms leads to consuming more acetate, then the release of electrons and the current generation will be increased, and in the end, more produced hydrogen will be attained.

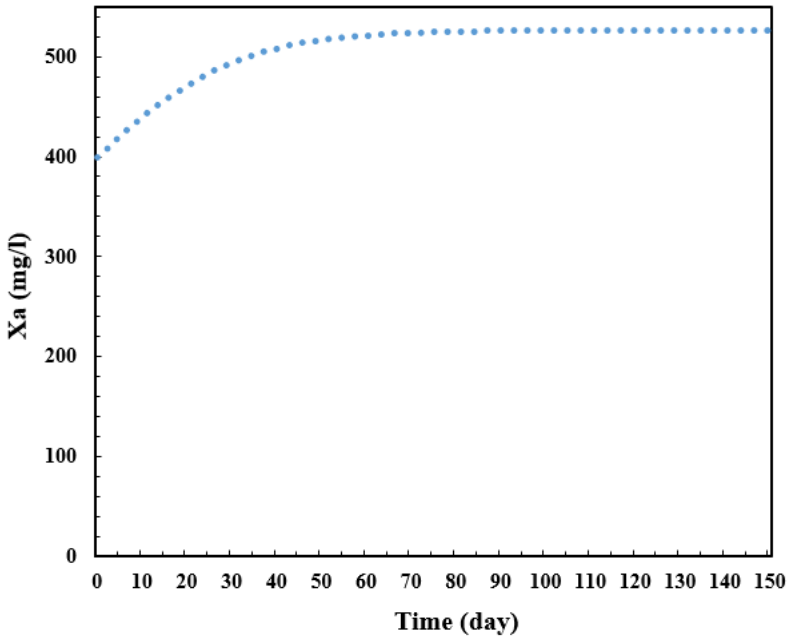


Figure 16. The behavior of anodophilic microorganisms (Xa).

Furthermore, the effect of anode surface area on hydrogen production rate has been investigated. Figure 17 indicates that more hydrogen will be produced by increasing the surface of the anode area because the biofilm covers the anode surface area, which is the main area of interaction between anodophilic bacteria and organic substrate to release electrons and protons before forming the hydrogen. Also, Figure 18 shows that the applied voltage directly affects current generation and hydrogen production rates in both types of MECs.

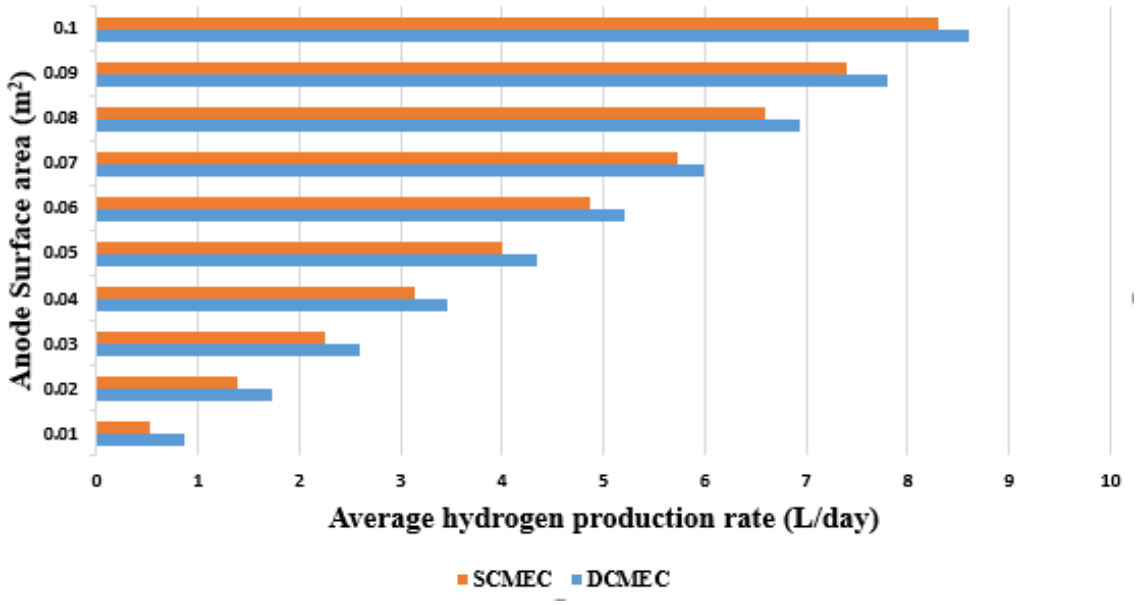


Figure 17. The effect of anode surface area on daily hydrogen production rates per liter of wastewater.

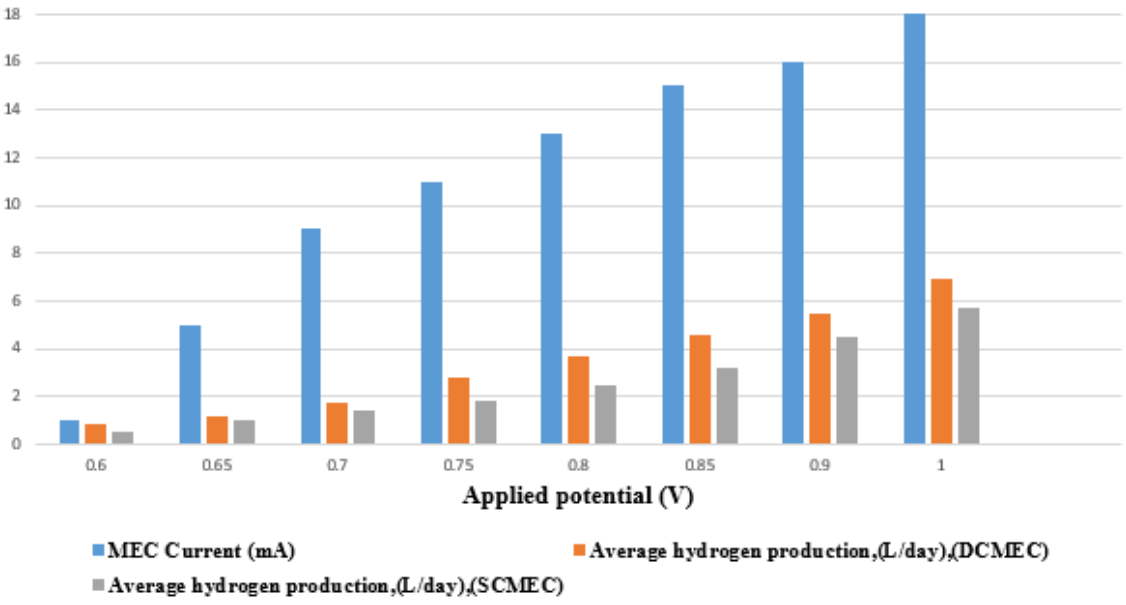


Figure 18. The effect of applied potential on MEC current and daily hydrogen generation per liter of wastewater.

4.2.2 Results of the MFC model

In this part, the behavior of anodophilic and methanogenic microorganisms has been investigated. Figure 19 and Figure 20 are shown that the activity of anodophilic increased over time, and methanogenic had more activity in the first days of the process. Also, as it appears in Figure 21, the voltage rose during the time, and it is due to the anodophilic population growth because more electrons will be released. Moreover, Figure 22 indicates the relation between power and current density. Corresponding to the results gained from this study and comparisons with the previous surveys, the average power generation per each m^3 of wastewater via MFC is estimated at about 0.033 kWh [140].

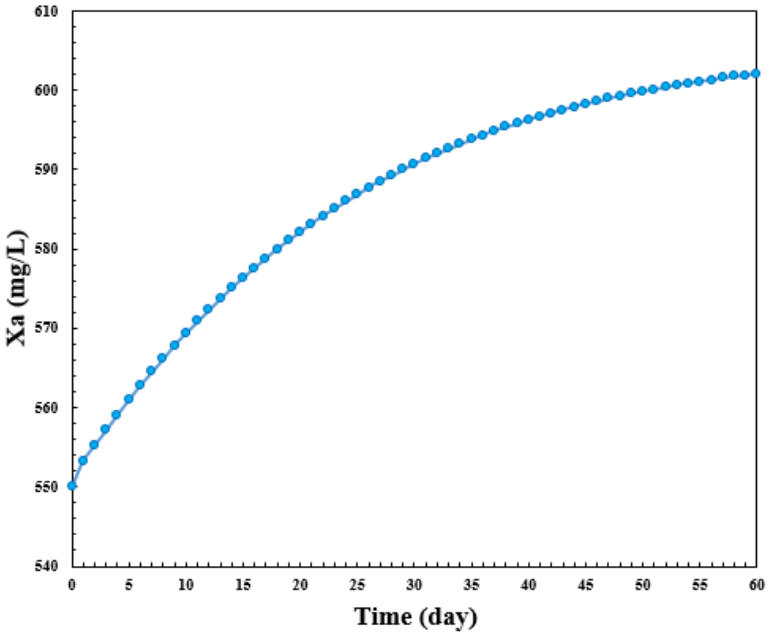


Figure 19. The behavior of anodophilic microorganisms (Xa).

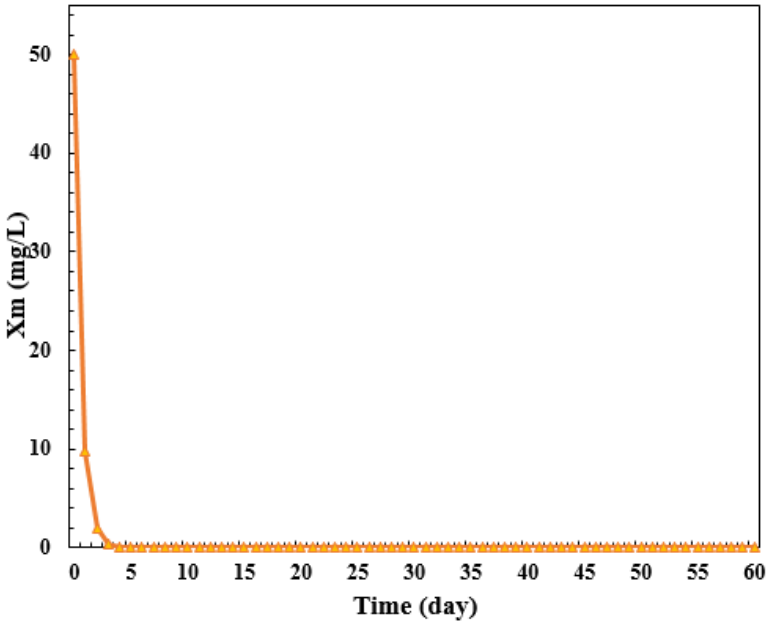


Figure 20. The behavior of methanogenic microorganisms (Xm).

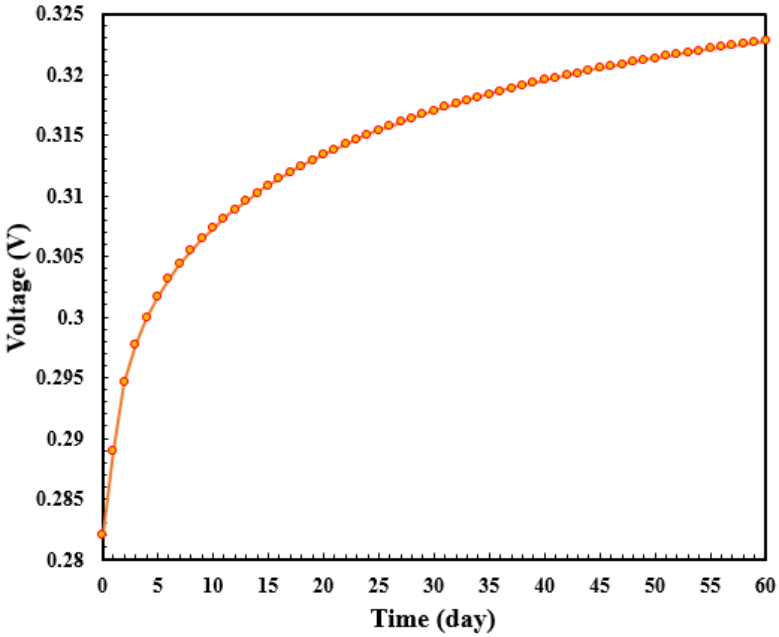


Figure 21. The output voltage of MFC.

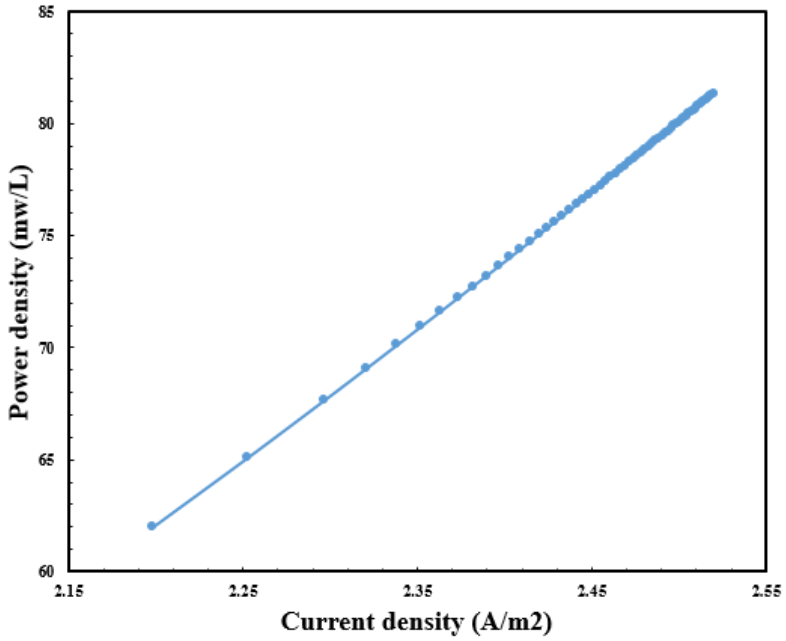


Figure 22. The relation between power density and current density.

4.3 Models application in real case studies:

In this section, the simulation codes and some literature data sets have been used to calculate the amount of hydrogen and power production for real case studies to know how microbial systems work on an urban scale for wastewater treatment and energy recovery. The schematic diagram of the proposed system is illustrated in Figure 23. based on the suggested system, wastewater should be collected in urban areas in the first step, then collected wastewater injected into the bio-electrochemical systems, including SCMEC, DCMEC, and MFC, to treat wastewater and generate hydrogen and electricity. In the first scenario, hydrogen as the main product of SCMEC and DCMEC can be considered a transportation fuel or feed of power or heating production technologies such as fuel cells and gas turbines. It should be noted that applied voltage can be covered by renewable sources of green electricity such as solar panels and wind turbines to run the MECs. In the second scenario power output of MFC can be used in two different applications, such as charging electric cars or directly used to cover a proportion of electricity demands of urban areas.

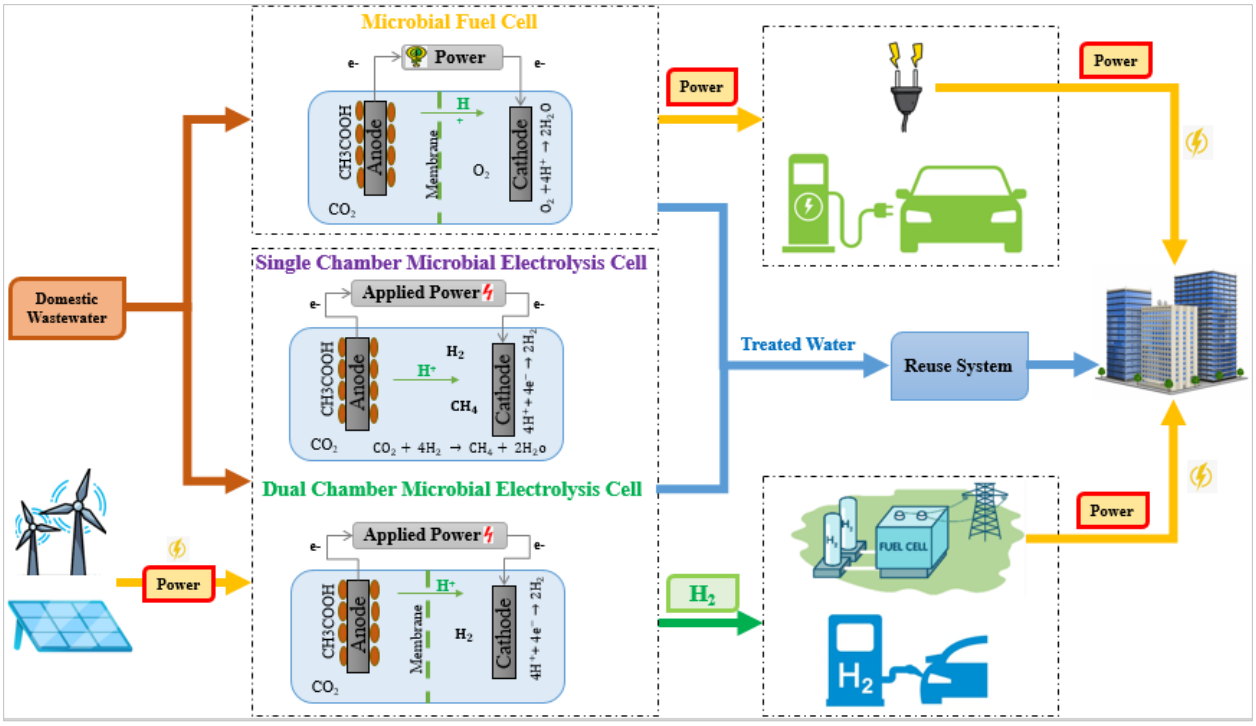


Figure 23. The schematic of microbial systems application in urban areas.

First scenario:

It aims to meet a proportion of local demands of six large mixed-use buildings located in Lachine East, Montreal, Canada (see Figure 24). It is assumed that the number of residents in this area is about 10,000 people. According to the assessment of drinking water use in Montreal, Canada, the average water consumption in residential sectors is around 300 l/day per capita [141]. Most of the research studies assume that the generated wastewater is equal to water consumption. Therefore, it is estimated that the region's total daily wastewater flow is about 3,000,000 L/day.

Then total wastewater is used individually as input for both types of MECs, including dual and single chambers. As a result, 141 kg/day and 230 kg/day are the value of produced hydrogen from SCMEC and DCMEC. Moreover, for running the MECs, electrical power is needed, which could be covered by wind turbines as green electricity generation systems. The required electricity for SCMEC and DCMEC systems is approximately 5,160 kWh [33]. The electricity for both of them is the same, but due to the activity of hydrogenotrophic bacteria, the hydrogen outputs from SCMEC are less than DCMEC.

Figure 24. The view of considered case study in Lachine East, Montreal, Canada.

Second scenario:

The second case study considered two non-domestic building blocks located at 4000 Saint Patrick Street, Montreal, Canada (see Figure 25). The average water consumption in non-residential buildings is less than that of residential buildings. So, 200 liters of wastewater per person and 375 building users are considered in this case study. The total daily wastewater generation used in bio-electrochemical reactors in this location is predicted to be 75,000 L/day. In this scenario, only MFCs are used as wastewater treatment technologies, producing electricity directly during the treatment process. The proposed model generated electricity via MFC in this location is about 2.5 kWh.

(A)

(B)

Figure 25. The geometry of C40 as a case study, rudimentary site view (A), designed and renovated blocks (B).

4.4 Comparison between the MFC and MEC:

As mentioned before, hydrogen is an ideal energy career. It contains 33.36 kWh of usable energy per 1 kg, approximately three times more than petrol and diesel. The previous part of the modeling reveals that 2.5 kWh will be attained by applying MFC as a wastewater treatment technology for the case study (second scenario). With the same wastewater input, the average hydrogen production is about 3.4 kg/day and 5.7 kg/day by applying single and dual chamber MECs. Also, the required electricity to run the SCMEC and DCMEC is 129 kWh. By considering all results above, Table 15 shows a rough calculation, including the energy content of generated hydrogen via MECs, and the potential of integrating the MECs with FC and MFC.in this study, 60% is the assumption for the efficiency of FC. According to Table 15, the power requirement for running the MECs is more than the generated power via FC. Extra electrical power is needed to use this technology as a wastewater treatment method and energy recovery. Other technologies like gas turbines and combustion engines use hydrogen to generate power and heat. They can be investigated in future steps and examine their efficiency and the amount of power generation with the same number used in this part to find the more efficient technologies to integrate with MECs. Also, the table below specified that the power generation via MFC is too small and less efficient than MECs.

Table 15. Power generation comparison (BESs).

Technology	Hydrogen production (kg)	Power consumption (kWh)	Energy contents (kWh)	Power generation via FC (kWh)
MFC	-	-	2.5	-
SCMEC	3.4	129	114	68.5
DCMEC	5.7	129	191	114.5

Note: the power generation numbers for MECs are based on the potential of using hydrogen from MECs as an input to other electricity generation technologies.

4.5 MEC vs. WE

Water electrolysis is one of the environmentally friendly technologies for pure hydrogen production. It needs only water and DC power from sustainable energy resources like MECs. There are some kinds of water electrolysis methods, including alkaline electrolysis (AE), Solid oxide electrolysis (SOE), and proton exchange membrane water electrolysis (PEMWE). In the anode chamber, water molecules split into oxygen, protons, and electrons. Then, the released electrons move to the cathode side through an external circuit and combine with protons to form the hydrogen gas. Among different types of WE methods, PEMWE is more favorable, which especially overcomes the drawbacks of AE. Some of the advantages of PEMWE are listed below:

I. Producing ultra-pure hydrogen
II. Compact design
III. High current density (above 2 A/cm^2)
IV. High efficiency
V. Fast response
VI. Small footprint
VII. Operate under low temperature (20-80 C)
VIII. Simple balancing of WPEM leads to be attractive for industrial application

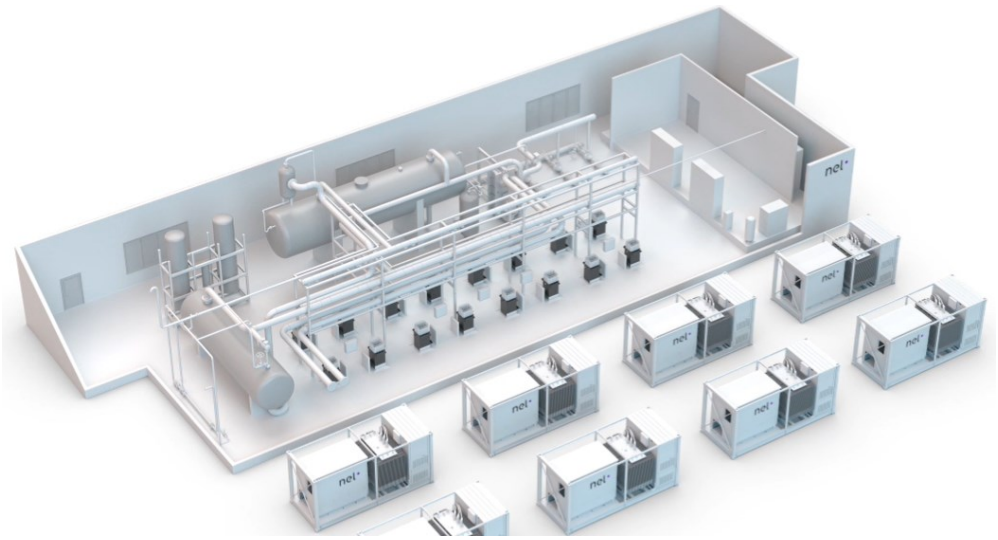


Figure 26. A general view of commercial proton exchange membrane water electrolyser [142]**.**

The chemical reaction at the anode and cathode chamber in PEMWE are as follows:

Anode chamber

$$2H_2O \rightarrow O_2 + 4H^+ + 4e^- \quad (63)$$

Cathode chamber

$$4H^+ + 4e^- \rightarrow 2H_2 \quad (64)$$

Overall reaction

$$2H_2O \rightarrow O_2 + 2H_2 \quad (65)$$

To the aim of this section, a comparison regarding hydrogen production in both types of MECs and PEMWE has been made. The results of this study reveal that for each cubic meter of wastewater, 0.077 kg H_2 and 0.046 kg H_2 can be generated via DCMEC and SCMEC, respectively. The below table compared the power consumption, water, and wastewater requirements for the generation of 1 kg hydrogen with MECs and PEMWE.

Table 16. The comparisons between MECs and PEMWE regarding one kg hydrogen production [143].

Method	DCMEC	SCMEC	PEMWE
Power consumption	24.5 kWh	30 kWh	51 kWh
Water requirement	-	-	0.009 m^3
Wastewater requirement	14.5 m^3	23m^3	-

According to the numbers provided in the above table, MECs consume less energy to produce 1kg of hydrogen than PEMWE. But, the volume of reactors would be bigger due to the required wastewater containing organic matter as the main substrate for hydrogen production.

4.6 Electricity consumption of BESs vs. WWTPs

WWTPs are known as huge energy consumer sectors. Besides, they have direct and indirect roles in increasing GHG emissions [144]. Hence, the measures related to reducing the energy consumption or energy recovery in the wastewater treatment process take place between the environmental specialists and researchers to shift towards the energy-positive WWTPs recently [145]. The energy consumption in WWTPs depends on several factors such as treatment methods and technologies, aeration systems, age and size of the plant, wastewater and sludge composition, wastewater flows, skills, and knowledge of operators [144]. Therefore, the data on energy consumption is different in each WWTP, as shown in Table 17. Also, the weather condition and

temperature have a minor impact on energy requirements through WWTP. For instance, a report has shown that the overall energy consumption in Canada with cold weather conditions was 0.3 kWh/m^3 while Singapore, located in tropical conditions, was 0.45 kWh/m^3 [144].

Table 17. The energy consumption in advanced WWTPs.

Location	Specific energy consumption (kWh/m^3)	Capacity of WWTPs (Based on the number of inhabitants)	Ref.
Poland (Rzeszow)	0.87	400,000	[146]
Poland (Slupsk)	0.48	250,000	[147]
Poland (Kronos)	0.67-1.11	117,000	[148]
Austria (Strass)	0.32	250,000	[149]
Italy (Turin)	0.3	2,700,000	[150]
Sweden (Stockholm)	0.48	500,000	[149]
China (Beijing)	0.26	2,400,000	[144]

Concerning energy reduction and energy production along with the wastewater treatment process, BESs such as DCMEC, SCMEC, and MFC are promising future technologies for extracting the energy from organic matter that exist in wastewater flows. Although pre-treatment and post-treatment steps are needed to be taken to achieve high-quality treated wastewater and different factors affect the required energy consumption via WWTPs and related systems, a rough estimation has been done in this part to compare the electrical power needed by BESs and conventional WWTPs. So following the energy consumption by applying mentioned technologies as wastewater treatment methods has been compared with the energy requirements in conventional WWTPs. Table 18 exhibits detailed comparisons between BESs and WWTPs. In addition, it should be noted that in both SCMEC and DCMEC, hydrogen and methane will be generated during the process that can be used as a source of energy. Regarding the MFCs, no input energies are needed to treat the wastewater, and electricity can be generated during the wastewater treatment process. As is shown in Table 15, the energy requirement in MECs is less than the energy contents of generated hydrogen through these systems. Therefore, SCMEC, DCMEC, and MFC can be considered energy-neutral or positive wastewater treatment technologies. It should be noted other facilities like pre-treatment and post-treatment systems may need to add MECs.

Table 18. Comparisons of electricity consumption by BESs vs. WWTPs.

Treatment method	Type of systems	Energy requirement (kW h/m^3)	Energy content (kW h/m^3)	Surplus energy production (kW h/m^3)
Conventional WWTPs	Centralized (Canada)	0.3	-	-
DCMEC	Decentralized	1.7	2.58	0.9
SCMEC	Decentralized	1.7	1.56	-0.14
MFC	Decentralized	-	0.033	0.033

4.7 Hydrogen-powered and electric car (HPC and EC)

Applying alternative green fuels or electrical powers as a driving force has become prominent for automobile manufacturers and environmental specialists in the last few years. Both HPC and EC have the potential to replace the old generation cars that work with petroleum, and they have less or zero CO_2 emissions to the environment. The most significant difference between the HPC and EC is that HPC work with hydrogen in a fuel cell system, and they produce electricity on their own. Figure 27 demonstrates a general view of fuel cell cars [151]. Also, HPCs fill up with hydrogen, which takes between 3-5 minutes for a full tank, i.e., much faster than electric car charging, and does not need external power sources [152]. Table 19 shows the hydrogen consumption in some fuel cell cars.

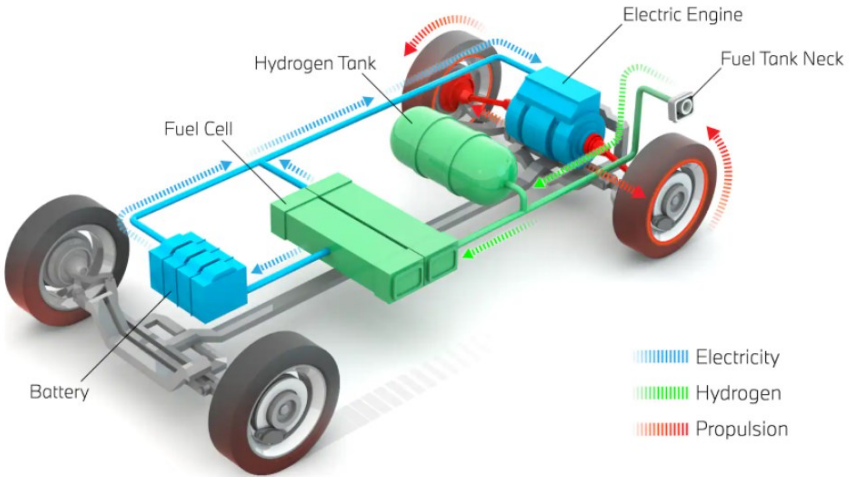


Figure 27. A view of Fuel cell systems in hydrogen-powered vehicles [151].

Table 19. Comparison between some kinds of fuel-cell cars with zero carbon emissions [153]**.**

Model	H_2 consumption (kg/100 km)	Tank capacity (kg)	Model	H_2 consumption (kg/100 km)	Tank capacity (kg)
Toyota MIRAI (second generation)	0.76	5.6	Hyundai NEXO	0.84	6.33
Mercedes-Benz GLC F-CELL	0.97	4.4	Hyundai ix35	1	5.64

Furthermore, it should be noted that ECs are limited by the range that they can travel because of the capacity of batteries. Battery charges can easily cover short trips, but they require long periods of recharging for longer road trips. The capacity of batteries varies in EC. They range from 33 kWh to 100 kWh in the Tesla Model S 100D [154]. Table 20 indicates the most popular and efficient EC in terms of kWh power consumption per 100 km driving with EC cars. It should be that the power consumption in the real world is dependent on ambient temperature, speed, and other factors, and the EC cars may consume more.

Table 20. The most efficient ECs in 2022 [155]**.**

Name of car	Power consumption (kWh /100km)	Name of car	Power consumption (kWh /100km)
Tesla Model 3, Standard Range Plus	14	Mini Electric	15
Fiat 500e	14	Seat Mii electric	15
Tesla Model 3, Long Range	14	Volkswagen e-up!	15
Hyundai Ioniq Electric	15	Smart EQ fortwo	15
BMW i3	15	Hyundai Kona Electric (39 kWh)	15.5

As it is mentioned in previous parts, the generated hydrogen and electricity from bio-reactors can be used in HPC and EC, respectively. So, according to the data provided in Table 20, it is assumed that 15 kWh [156] is an average energy consumption per 100 km by EC, and 0.9 kg hydrogen is

needed to drive 100 km with HPC. In the next table, the number of people or total wastewater as a feed for BESs and their power consumption is determined to show how BESs work to generate the fuel for driving 100 km with EC and HPC.

Table 21. The estimation of using the generated hydrogen and power via BESs as fuel in green cars.

Type of green car	The required energy by green cars to drive 100 km	Selected BESs	Total wastewater	Energy consumption by BESs
EC	15 kWh	MFC	455 m^3	-
HPC	0.9 kg H_2	DCMEC	13 m^3	22.5 kWh
HPC	0.9 kg H_2	SCMEC	21 m^3	27 kWh

4.8 Conclusion:

This study has modeled three wastewater treatment and energy recovery technologies, including MFC, SCMEC, and DCMEC. All models were implemented using the Python programming language. The Radau methods applied to solve ODE equations were different from previous research. Then, the model was validated with the works of former researchers successfully. Two models of SCMEC and DCMEC were compared, and it is shown that DCMEC is able to generate more hydrogen than SCMEC. Because there is a membrane between the anode and cathode chamber, and it is permeable only against protons, the hydrogen is produced in the cathode chamber without the existence of hydrogenotrophic bacteria that consume the generated hydrogen and CO_2. Also, the sensitivity analysis in this research reports that the greater anode surface area and applied potential in MECs will increase the hydrogen production rate. The results from this research model in MFCs also show that:

- The activities of anodophilic and methanogenic bacteria in MFCs are the same as in MECs.
- The voltage increases over time.
- There is a linear relationship between power density and current density.

The next contribution of this thesis was to examine the mentioned technologies on urban scales by applying the models to two real case studies. The application of MECs and MFCs as advanced wastewater treatment methods was investigated in the first (residential area) and second (commercial buildings) case studies. Then, comparisons have been made between SCMEC, DCMEC, and MFC based on the data extracted from the second case study. The comparisons

reveal that the system containing MECs integrated with fuel cells can generate more power than MFCs.DCMEC and SCMEC are most feasible and cost-effective than MFCs.

Moreover, the electrical energy consumption for the wastewater treatment via conventional WWTPs vs. BESs has been compared. The results show that the overall process in BESs needs less electrical energy to treat the wastewater. In some cases, they can be accounted for as energy-positive technologies for wastewater treatment if more efficient technologies than FC are integrated with MECs to generate power and heating. Also, WE have been compared with both types of MECs regarding hydrogen production and power consumption. The results reveal that MECs consume less power but need a considerable amount of wastewater to consume their soluble organic matters, but in WE, only 9 liters of water can generate 1 kg of hydrogen. In the final step, the capability of utilizing the generated hydrogen and power through BESs as a transportation fuel has been investigated. The outcome shows the driving distance that EC and HPC can reach with green fuels from BESs.

Future works like the integration of fuel cells, wind turbines, solar panels, compressors, storage systems, or any other types of equipment models are necessary to know how these systems work from the first user to the end-users. Above and beyond, pre-treatment and post-treatment systems should be designed to calculate the whole energy needed to treat the wastewater with BESs. Then the cost analysis in the next steps is extremely important to choose the best option for wastewater treatment. In addition, the potential of integration of MFC as a source of electrical power for MEC can be surveyed to have a mix of microbial systems for wastewater treatments. Bio-electrochemical systems are new, and more comprehensive research and analysis need to be taken to have a commercial model. More parameters and conditions should be considered to increase efficiency and decrease the operation and construction costs. To better evaluate the integration into urban case studies, the exact number of residents and daily wastewater flow in each area should be addressed to obtain trustable results.

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