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Mathematical Modeling of Microbial Electrolysis Cells for Enhanced Urban Wastewater Treatment and Hydrogen Generation

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Abstract: Conventional wastewater treatment plants (CWTPs) are intensive energy consumers. New technologies are emerging for wastewater treatment such as microbial electrolysis cells (MECs) that can simultaneously treat wastewater and generate hydrogen as a renewable energy source. Mathematical modeling of single and dual-chamber microbial electrolysis cells (SMEC and DMEC) has been developed based on microbial population growth in this study. The model outputs were validated successfully with previous works, and are then used for comparisons between the SMEC and DMEC regarding the hydrogen production rate (HPR). The results reveal that the daily HPR in DMEC is higher than in SMEC, with about 0.86 l H_2 and 0.52 l H_2, respectively, per 1 L of wastewater. Moreover, the results have been used to compare the HPR in water electrolysis (WE) processes and MECs. WE consume 51 kWh to generate 1 kg of hydrogen, while SMEC and DMEC require only 30 kWh and 24.5 kWh, respectively.

Keywords: microbial electrolysis cell; hydrogen; wastewater; modeling

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1. Introduction

Population growth, rapid urbanization, and the human desire to improve their living standards lead to increased energy demands in four main sectors: power, buildings, industry, and transport [1]. Today's energy systems are severely dependent on fossil fuels, and the depletion of non-renewable resources in parallel with increasing rates of greenhouse gas (GHG) emissions has become one of the main concerns [2]. Therefore, research into renewable energy generation sources to transform cities and industries towards fully sustainable energy systems is increasing exponentially [3]. Currently, there is no single source of renewable energy that can replace the whole conventional fossil fuel energy source, however combining renewable, clean, and long-lasting energy sources such as biomass, solar, wind, geothermal, hydroelectricity, wave, and hydrogen may address the energy demands and preserve the environment in the future. Hydrogen is an ideal alternative to replace traditional fossil fuels as a clean (carbon emission-free) and sustainable energy career for driving energy systems [4–6]. Hydrogen is recognized as the lightest, and most abundant chemical substance in the universe. It is a kind of clean and carbon-neutral source of energy because the sole by-product of hydrogen combustion is water [2]. Hydrogen has a high energy density of around 120 MJ/kg, and 33.6 kWh of usable energy per kg in terms of electrical energy which is three times more than gasoline [3,7]. Hydrogen has applications in various sectors, such as transportation through electric cars, electricity, and heating generation via fuel cells. Moreover, it could be added or used as a composition to produce other enriched energy mixtures such as ammonia and methanol [8]. Various pathways to produce hydrogen are classified according to their applications and sources, such as WE, gasification, PV-electrolysis, dark fermentation, coal gasification, and fossil fuel reforming [9,10].

Moreover, in recent years, large amounts of wastewater have been produced yearly, and the emission of wastewater in the world is increasing. Recovering the chemical energy of wastewater is meaningful, and the demand for new and efficient technology in wastewater treatment has become urgent [11,12]. Freshwater availability is predicted to decrease by 40% in the next decades [13].

Among several types of hydrogen production methods, bio-electrochemical systems (BECs), such as MECs, are a promising technology for wastewater treatment and hydrogen production simultaneously [14]. MECs consist of a microbial anode and conventional cathode electrodes, substrates, ion exchange membranes, and microorganisms [15]. Microorganisms exist in an anode chamber, and they need the culture medium necessary for their growth and forming the biofilm at the anode surface area, which is the main part of the MECs to degrade carbon substrates and electrons transferring. In an anode chamber, organic matters oxidize and release protons and electrons that transfer to the cathode side through an external circuit. Protons penetrate via a membrane to the cathode chamber [16]. Moreover, anaerobic conditions and external voltage are needed in the cathode chamber to reduce protons for hydrogen production [17]. There are two types of MECs, including SMEC and DMEC. In DMEC, a proton exchange membrane (PEM) prevents the wastewater solution from transferring the anode to the cathode chambers and reduces the hydrogen diffusion from the cathode to the anode resulting in increased pure hydrogen. Although some researchers [18–20] observed the pilot scale of MECs and calculated main objectives such as organic load, applied voltage, temperature, inoculum, and pH experimentally, the other ones [21–24] prioritized analytical solutions to optimize operational conditions including physical, chemical, and biological properties for increasing hydrogen production rate and improving wastewater treatment process. In this regard, Pinto et al. [21] conducted a mathematical model for a continuous operation MEC reactor fed with synthetic wastewater where acetate was the primary substrate in the dilution. The model was dynamic, and multi-population microbial growth, including three different microbial populations, was considered in their assumption. Their critical research point was the effect of voltage and organic load ratio on hydrogen production. The final output agreed with the experimental data, and the maximum hydrogen production rate and desired chemical oxygen demand (COD) level were achieved. A MATLAB-based MEC model simulated by Gonzalez et al. [24] investigated different parameters such as microbial growth and competition on acetate consumption in wastewater flow, electrical current generation, and hydrogen production. Two primary control approaches were used, including dilution rate and applied potential assumed in the mathematical model to optimize and improve the hydrogen generation rate. The measured results showed that both control laws 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 latter were feasible for a short and long period of time, respectively. Furthermore, Estrella et al. [23] proposed a dynamic mathematical model resulting from the mass balance of continuous flow MECD. According to the author's investigation, the ordinary differential equations (ODEs) introduced the model, and steady-state analysis determination concluded that only one of the three possible steady states was stable. Moreover, they compared two microbial populations and proved that their concentration substantially impacted hydrogen and methane production rates, especially during the initial stages of the MEC. Process optimization presented in the proposed model applies to off-line processes and real-time process control.

This study has conducted mathematical modeling of SMEC and DMEC to treat wastewater and energy recovery on urban scales. As shown in Figure 1, decentralized energy systems running on renewable sources would be the advanced pathway to treat domestic wastewater and energy production simultaneously. The proposed innovative cycle includes microbial electrochemical reactors, pre- and post-treatment systems, sustainable energy sources, and fuel cells. Since organic matter is supplied by domestic wastewater, after collecting generated wastewater and conducting pre-treatment, the influent injects into the reactors, producing pure hydrogen. Then, hydrogen is converted to electrical energy via fuel cells. At the same time, post-treatment will apply to treated water to meet the water quality standard for urban area purposes. Therefore, generated power could compensate for a proportion of the electricity demands in urban areas. In addition, treated water could be reused for different purposes, like cleaning and toilet flushing irrigation, decreasing pressure on freshwater resources and water treatment plants.

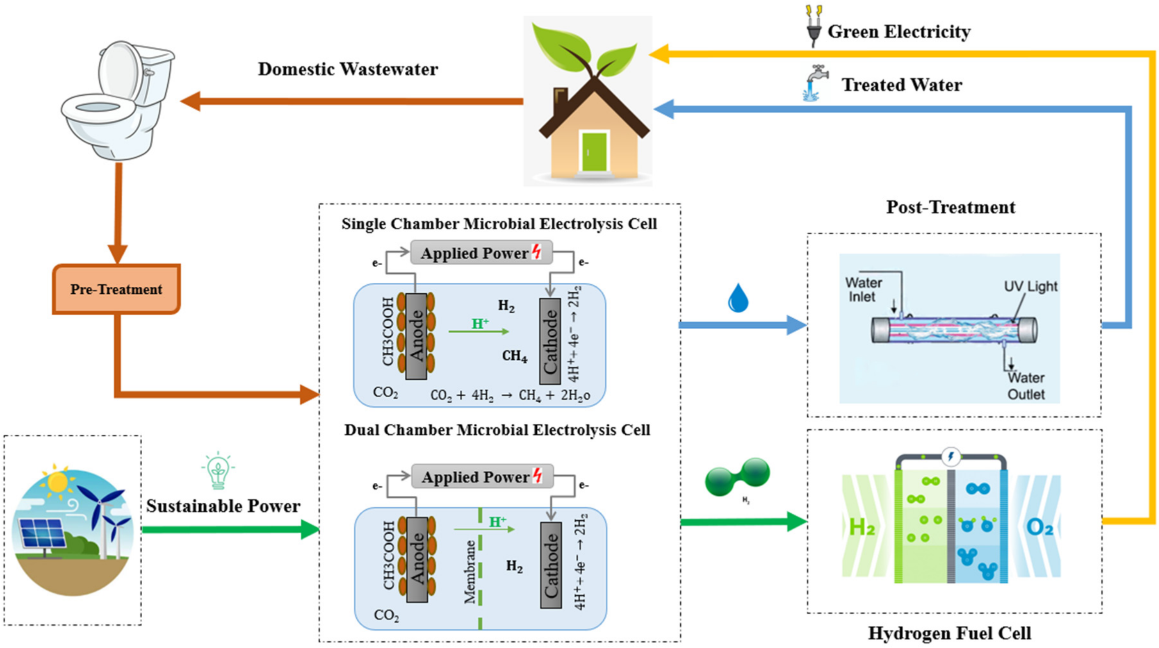

Figure 1. Advanced wastewater treatment and energy recovery cycle.

The thermodynamic modeling of the onsite hybrid system is developed in Python as a high-level programming language, and the Radaue method is applied as a numerical solution to solve the ordinary differential equations (ODE), which is different from previous studies. Both types of MECs have been modeled in this investigation to compare their efficiency as wastewater and energy recovery methods.

A real case study with six residential building complexes and 10,000 inhabitants located in Lachine East, Montreal, Canada was used to apply the models to an urban setting (see Figure 2). Based on the Montreal data sets, the water consumption for each person is about 300 L/day [25]. Therefore, a total daily wastewater flow of (3,000,000 L/day) has been assumed to examine the potential of decentralized wastewater treatment in urban areas. Then, the HPR is compared between two types of MECs. In addition, the energy consumption and HPR by MECs have been compared to CWTPs and WE, respectively.

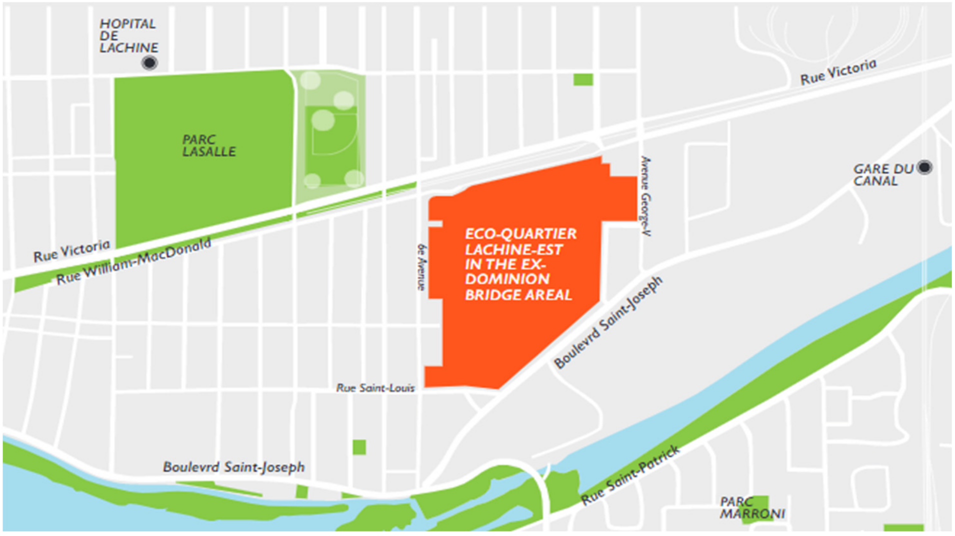

Figure 2. Location of the considered eco-district case study in Lachine East, Montreal, Canada.

2. Materials and Methods

2.1. Model Description of Microbial Electrolysis Cells (MECs)

The proposed model for SMEC and DMEC in this study has been adapted from Gonzalez et al. [24]. The presented model is a continuous system considering the activities of three microbial populations, including anodophilic, methanogenic, and hydrogenotrophic bacteria. The anodophilic degrades the acetate as the main carbon source with the amount of 550 mg/L of wastewater (Lw) to release the electrons, protons, and CO_2. Moreover, methanogenic bacteria use acetate to form methane and CO_2. Hydrogentrophic, as undesired bacteria, reacts with mineralized carbon (CO_2) and hydrogen to shape the methane, and they decrease the level of HPR. Figure 3 depicts a general schema of SMEC and DMEC regarding the interaction between microorganisms and substrates in wastewater solution. Furthermore, intracellular and extracellular mediators are assumed to transfer electrons from anodophilic bacteria to the anode surface and from the anode to the cathode electrode through the external circuit, respectively. Some essential indicators, including pH, temperature, and pressure, are constant during the chemical processes in both types of MECs. In existing BECs, where substrate gradient in the biofilm is neglected, the uniform distribution of microbial populations and ideal mixing is assumed in the anode part.

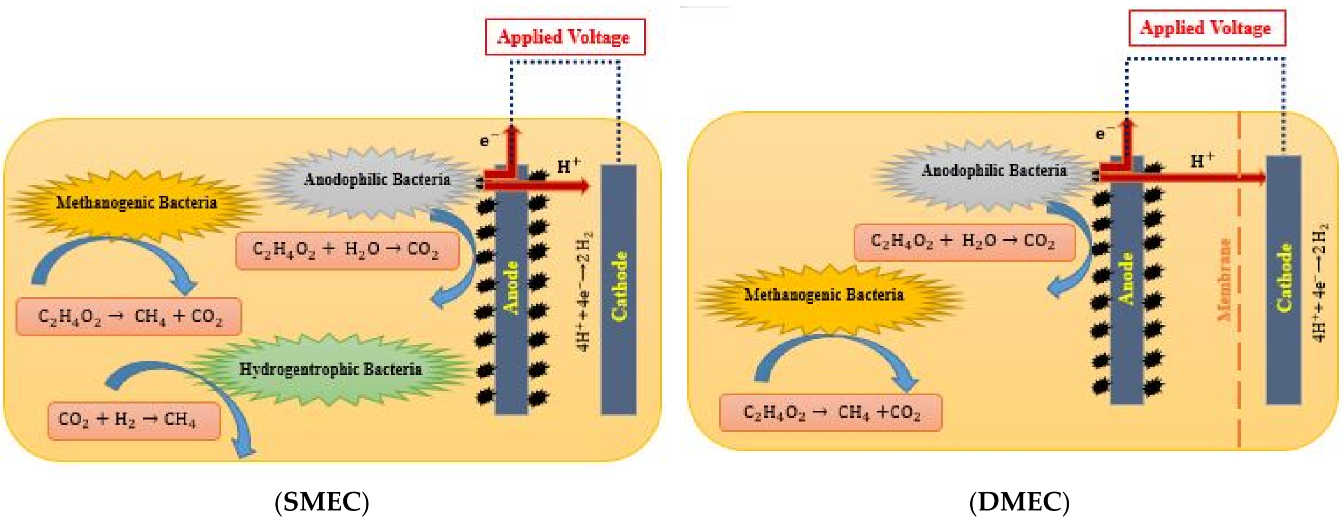

Figure 3. A view of microbial activities in the anode compartment.

2.2. Equations for Modeling of SMEC and DMEC

In this section, all mathematical equations for modeling two MEC configurations (single and dual) are categorized. The mathematical modeling of SMEC and DMEC is implemented in Python. Initial value problems for stiff ordinary differential equations (SODEs) occur very frequently in different situations such as biology and chemical processes [26]. Since the Radau IIA as a numerical method is reliable, accurate, and stable, the mentioned approach is applied in the present research to solve proposed SODEs in the Mass Balance Section. The Radau method is one of the kinds of implicit Runge-Kutta schemes, and it has been successfully applied to SODEs because of its strong algorithm [27].

2.2.1. Chemical Reactions at Electrodes

- SMEC

Anode chamber

$$C_2H_4O_2 + 2H_2O + 4M_o \rightarrow 4M_r + 2CO_2 \tag{1}$$

$$4M_r \rightarrow 4M_o + 8e^- + 8H^+ \tag{2}$$

$$CO_2 + HCO_3^- + 8e^- + 8H^+ \rightarrow CH_3COO^- \tag{3}$$

Cathode chamber

$$C_2H_4O_2 \rightarrow 4CH_4 + CO_2 \tag{4}$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2 \tag{5}$$

$$2H_2O + 2e^- \rightarrow 2OH^- + H_2 \tag{6}$$

- DMEC

Anode chamber

$$C_2H_4O_2 + 2H_2O + 4M_o \rightarrow 4M_r + 2CO_2 \tag{7}$$

$$4M_r \rightarrow 4M_o + 8e^- + 8H^+ \tag{8}$$

$$C_2H_4O_2 \rightarrow 4CH_4 + CO_2 \tag{9}$$

Cathode chamber

$$2H_2O + 2e^- \rightarrow 2OH^- + H_2 \tag{10}$$

2.2.2. Mass Balance Equations

In this study, acetate is considered the primary substrate in wastewater solutions. The mass balance equations for the continuous reactors of both SMEC and DMEC are described as follows, where S (mg S/L) is defined as the acetate concentration. Moreover, the concentration of anodophilic and methanogenic microorganisms are represented as X_a and X_m, respectively (mg X/L). D stands for dilution rate which is equal to 1 (1/d) in this work.

$$\frac{dS}{dt} = D(S_0 - S) - q_a X_a - q_m X_m \tag{11}$$

$$\frac{dX_a}{dt} = \mu_a X_a - K_{d,a} X_a - \alpha_1 D X_a \tag{12}$$

$$\frac{dX_m}{dt} = \mu_m X_m - K_{d,m} X_m - \alpha_1 D X_m \tag{13}$$

All the above equations are applied for both types of MECs, but in SMEC, because of the existence of hydrogenotrophic microorganisms, one more equation should be added to the Mass Balance Section shown below. α_1 and α_2 are dimensionless biofilm retention constants, and the assumed value for them are 0.5410 and 0.4894, respectively.

$$\frac{dX_h}{dt} = \mu_h X_h - K_{d,h} X_h - \alpha_2 D X_h \tag{14}$$

2.2.3. Hydrogen Production Rate

The hydrogenotrophic microorganism in the anode chamber is the only difference between SMEC and DMEC models. Therefore, their presence at SMEC leads to two different hydrogen production rates, as appears below.

- SMEC

$$Q_{H_2} = Y_{H_2} \frac{I_{MEC}}{mF_1} \frac{RT}{P} - Y_h \mu_h X_h V_r \tag{15}$$

- DMEC

$$Q_{H_2} = Y_{H_2} \frac{I_{MEC}}{mF_1} \frac{RT}{P} \tag{16}$$

2.2.4. Intracellular Mass Balance

For each electrogenic microorganism, the balance equation should be written as below, and the total mediating fraction (M_{total}) is about 1000 (mg M/mg X).

$$M_{total} = M_r + M_o \tag{17}$$

$$\frac{dM_o}{dt} = \frac{\gamma}{V_r X_a} \frac{I_{MEC}}{mF_1} - Y_M q_a \tag{18}$$

M_r and M_o are the concentration of reduced and oxidized forms of the intracellular mediator (mg M/mg X).

2.2.5. Microbial Kinetic

μ_a and μ_m are the growth rate of anodophilic microorganisms and acetoclastic methanogenic microorganisms, respectively. q_a and q_m are the anodophilic microorganisms and acetoclastic methanogenic substrate consumption.

$$\mu_a = \mu_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_{MEC} + M_o} \tag{19}$$

$$\mu_m = \mu_{max,m} \frac{S}{K_{s,m} + S} \tag{20}$$

$$q_a = q_{max,a} \frac{S}{K_{s,a} + S} \frac{M_o}{K_{MEC} + M_o} \tag{21}$$

$$q_m = q_{max,m} \frac{S}{K_{s,m} + S} \tag{22}$$

The maximum value of μ_a, μ_m, μ_h, q_a and q_m are the constant numbers as they are mentioned below:

$\mu_{max,a}$ = 1.97 (1/d); $\mu_{max,m}$ = 0.3 (1/d); $\mu_{max,h}$ = 0.5 (1/d); $q_{max,a}$ = 13.14 (mg S/mg X d); $q_{max,m}$ = 14.12 (mg S/mg X d).

Due to the absence of a membrane in SMEC, μ_h is referring to the growth rate of hydrogenotrophic microorganisms.

$$\mu_h = \mu_{max,h} \frac{[H_2]}{K_h + [H_2]} \tag{23}$$

2.2.6. Electrochemical Equations

The external voltage E_{app} needed to run the MECs can be calculated via the below equation, where E_{CEF} is the value of electrode potential. The assumed numbers for E_{app} and E_{CEF} are about 0.6 (V) and −0.35 (V), respectively.

$$E_{app} = E_{CEF} - \eta_{ohm} - \eta_{conc} - \eta_{act} \tag{24}$$

The ohmic (η_{ohm}), concentration (η_{conc}), and activation (η_{act}) losses at the anode chamber are calculated by use of the below equations.

$$\eta_{ohm} = R_{int} I_{MEC} \tag{25}$$

$$\eta_{conc} = \frac{R_1 T_{MEC}}{mF} ln(\frac{M_T}{M_r}) \tag{26}$$

$$\eta_{act} = \frac{R_1 T_{MEC}}{\beta mF} sinh^{-1}(\frac{I_{MEC}}{S_A i_0}) \tag{27}$$

The MECs current is calculated as follows:

$$I_{MEC} = E_{CEF} + E_{app} - \frac{R_1 T_{MEC}[ln\left(\frac{M_T}{M_r}\right) + \frac{1}{\beta} sinh^{-1}(\frac{I_{MEC}}{S_A i_0})]}{R_{int}} \tag{28}$$

In the below equation, internal resistance, which is liked to electrogenic, can be calculated, and the dedicated numbers for R_{MIN} and R_{MAX} are 2 (Ω) and 200 (Ω), respectively.

$$R_{int} = R_{MIN} + (R_{MAX} - R_{MIN}) e^{-k_R X_a} \tag{29}$$

2.3. Desing Parameters

All parameters that are needed for simulation are shown in Table 1. The mentioned parameters are extracted from the works of Estrella et al. [23] and Gonzalez et al. [24].

Table 1. Modeling parameters for two types of MECs.

Parameters	Description	Value and Units
$[H_2]$	Dissolved hydrogen saturated concentration	1.5 (mg/L)
K_h	Half–rate constant for hydrogenotrophic microorganisms	0.001 (mg/L)
K_R	Constant, which determines the slope of the curve in the equation	0.024 (L/mg X)
$K_{d,a}$	The decomposition rate of anodophilic microorganisms	0.04 (1/d)
$K_{d,h}$	The decomposition rate of hydrogenotrophic microorganisms	0.01 (1/d)
$K_{d,m}$	The decomposition rate of methanogenic microorganisms	0.01 (1/d)
$K_{S,a}$	Half–rate (Monod) constant for anodophilic microorganisms	20 (mg S/L)
$K_{S,m}$	Half–rate (Monod) constant for methanogenic microorganisms	80 (mg S/L)
K_{MEC}	Half–rate constant for the oxidized intracellular mediator	0.01 (mg M/L)
Y_h	The yield rate for hydrogen-consuming methanogenic microorganisms	0.05 (ml H_2/mg X)
Y_{H_2}	Hydrogen yield	0.9
Y_M	The yield rate for the oxidized mediator	3.3 (mg M/mg A)
β	Oxidation transfer coefficient or reduction	0.5
γ	Mediator molar mass	663,400 (mg M/mole M)

3. Results and Discussion

3.1. Model Validation

The validation of a mathematical model of a dynamic structural system is another crucial step that entails the comparison of predictions from the model to measured results from experiments. Hence, the final calculated results compared with the work of Gonzalez et al. [24]. According to Figures 4 and 5, at the anode side, the behaviour of methanogenic (*Xm*) and hydrogenotrophic (*Xh*) microorganisms is fully validated. Both figures demonstrated that at an earlier time when the process started, the existence of methanogenic and hydrogenotrophic microorganisms was at the highest level, then by passing time, reduced to reach a value of zero. In contrast, the activity of anodophilic (X_a) at the start point of the process is zero, but it is raised fast before day ten and reaches the maximum value, which leads to generating hydrogen, according to Figure 6. Generally, the mentioned figures show that the competition is won by anodophilic microorganisms, which release protons and electrons from the hydrogen. The remaining microorganisms are undesired bacteria, including methanogens (X_m) and hydrogenotrophic (X_h). As the methanogens (X_m) consume acetate to generate CO_2 and methane, the hydrogenotrophic (X_h) use produced hydrogen and CO_2 to form methane, resulting in decreased hydrogen purity.

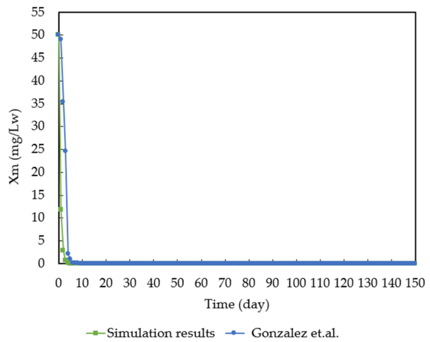

Figure 4. The behavior of (X_m) validation [24].

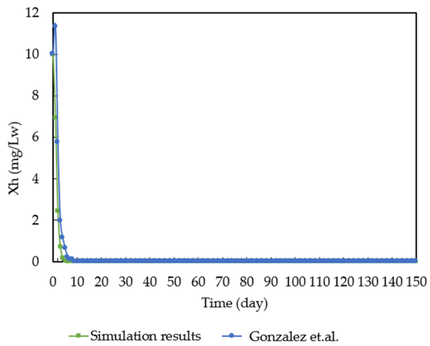

Figure 5. The behavior of (X_h) validation [24].

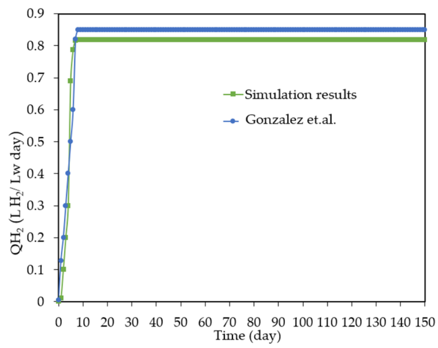

Figure 6. Validation of (QH_2) [24].

3.2. HPR in DMEC vs. SMEC

In this study, the MECs models deliver the HPR within SMEC and DMEC, which is approximately 0.52 L H_2 gas/Lw day and 0.86 L H_2 gas/Lw day, respectively. At the SMEC, there is no membrane between the anode and cathode compartment, so it lets the hydrogenotrophic microorganisms consume generated hydrogen, which leads to a decrease in the level of HPR in SMEC. Nevertheless, at DMEC, the cathode side helps the system have more hydrogen than SMEC, as illustrated in Figure 7. Hence, it could be concluded that although SMEC reduces the cost of construction and operation and, in some cases, needs less power than DMEC, it has a lower HPR.

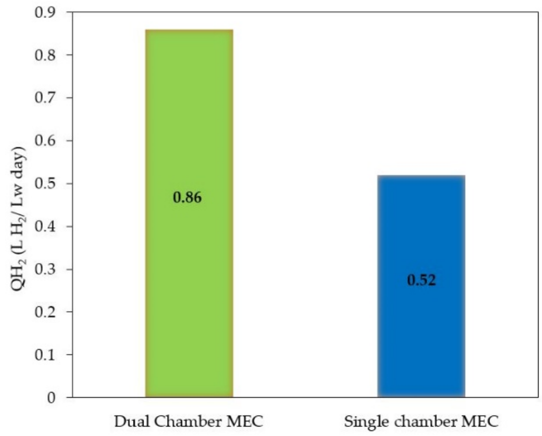

Figure 7. The comparison between single and dual chamber MEC regarding the generated hydrogen.

3.3. Sensitive Analysis

This part investigates the effect of the anode surface area and applied potential on HPR. The impact of applied voltage and anode surface area on hydrogen production rate are two key parameters. So, Figures 8 and 9 have been added to this research to present the sensitivity analysis. Figure 8 depicts that more hydrogen could be produced by expanding the anode surface area. Since biofilm covers the anode surface, and it is the primary area of interaction between anodophilic bacteria and acetate, adding more to that area concludes more chemical reactions and releases more electrons and protons before generating the hydrogen. Moreover, Figure 9 demonstrates that by rising the applied voltage, the hydrogen production rates are directly affected in both types of MECs.

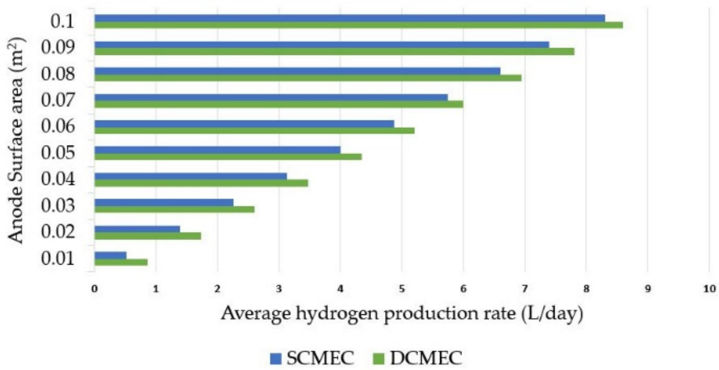

Figure 8. The effect of anode surface area on hydrogen production rates.

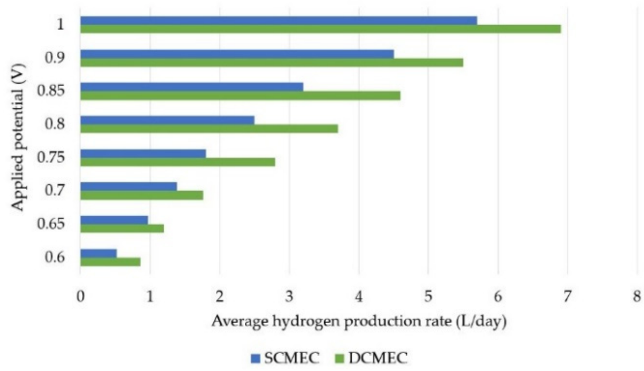

Figure 9. The effect of applied potential on current and hydrogen generation.

3.4. Case Study

For another goal of this study, the simulation codes have been used to calculate the HPR by applying wastewater treatment technologies on the urban scale. Therefore, according to the information provided in the Case Study Section, the 3000 m^3/day of wastewater flow is used as an input for both types of MECs, including dual and single chambers. Based on the mathematical model, the DMEC and SMEC are able to generate 0.077 kg H_2 and 0.046 kg H_2 per cubic m^3 of wastewater. Hence, 141 kg H_2/day and 230 kg H_2/day are the average value of produced hydrogen from SMEC and DMEC individually in the location of the mentioned case study.

Moreover, because Gibbs free energy on chemical reactions of MECs, those are not thermodynamically favorable. So, external input energy is needed to proceed with the chemical process prior to generating the hydrogen. Although the power consumption in MECs is less compared to other technologies such as WE, optimization is still needed to reach a cost-effective and reliable process. In this regard, pH is one of the key points affecting power consumption in MECs. At a lower pH, power consumption can be reduced. However, it should be noted that low pH has drawbacks for microbial activities, so finding the optimal level for pH is one of the important milestones to reaching out to the conventional MECs [18]. Since carbon neutral and green energies have been prominent in recent years, the energy required by MECs can be covered by renewable resources such as wind turbines and solar panels. Based on the hydrogen production values, the total required electricity is predicted to be about 5160 kWh per day for both types of MECs. Although SMEC and DMEC consume the same power, SMEC generates less hydrogen than DMEC, which is the consequence of hydrogenotrophic bacteria activities.

4. CWTPs vs. MECs

The energy intensity of CWPT makes researchers transform the CWTP into an energy-positive industry by applying advanced technologies for both treatment and energy production. The energy consumption in CWTPs varies depending on several features such as treatment methods and technologies, aeration systems, age and size of the plant, wastewater flows, the composition of sludge and wastewater, and the weather condition has a minor impact [28]. According to evidence, the average power consumption in CWTPs in Canada is approximately 0.3 kWh/m^3 [28]. Table 2 compared the energy required for treating one cubic meter of wastewater through CWTPs, SMEC, and DMEC. It is shown that by considering the advantages of energy production via MECs at the end of applying MECs instead of CWTPs as wastewater treatment methods, less energy is needed to treat the sewage. Moreover, in some cases, MECs generate more energy than they consume, i.e., they can be considered as positive energy technologies for treating wastewater.

Table 2. The comparison of electricity consumption by MECs vs. CWTPs.

Treatment Method	Energy Requirement	Energy Content	Surplus Energy Outputs
CWTPs	0.3 kWh/m^3	-	-
DMEC	1.7 kWh/m^3	2.58 kWh/m^3	0.9 kWh/m^3
SMEC	1.7 kWh/m^3	1.56 kWh/m^3	−0.14 kWh/m^3

5. WE vs. MECs

WE is an electrochemical process that uses electrical power to split water molecules into hydrogen and oxygen. No pollution or CO_2 emissions are released during this process, and it can be well-suited for small-scale and large-scale renewable hydrogen production. In this section, a comparison regarding hydrogen production and power consumption between both types of MECs and WE have been made. Table 3 reveals that WE needs more energy to generate 1 kg H_2, but the reactor capacity is less than MECs. As proof to validate the below results, it should be mentioned that in MECs, the oxidation of organic compounds is replaced by water oxidation in WE, leading to lower redox potential and thermodynamic cell voltage of a MEC decrease according to the mentioned concept. So, power consumption by MECs is less compared to WE in standard conditions. Moreover, it should be noted that applying MECs is not only a hydrogen production method; they can also treat the wastewater during the hydrogen production process, and then treated water can be used in different applications such as toilet flushing, irrigation, and carwashes.

Table 3. One kilogram of hydrogen production in both types of MECs compared to WE.

Technology	Energy Consumption for 1 kg H_2 Production	Pure Water Requirement	Wastewater Requirement
WE	51 kWh	0.009 m^3	-
DMEC	24.5 kWh	-	14.5 m^3
SMEC	30 kWh	-	23 m^3

6. Conclusions

This study analyzed the performance of microbial electrolysis cells for the simultaneous treatment of wastewater and hydrogen generation. It successfully applied the Radaue method for solving SODEs equation, and the mathematical modeling of SMEC and DMEC shows a good agreement with the literature data. The comparison regarding hydrogen production rate indicates DMEC generates more hydrogen than SMEC, and they consume the same power due to the activity of the hydrogenotrophic bacteria. The figures and analysis show that expanding the anode surface area or leveling the applied voltage directly affects the hydrogen production rate.

Moreover, the results express that SMEC and DMEC consume less energy than conventional wastewater treatment plants, and they can be considered a decentralized treatment method in urban areas without the necessity of expensive piping and pumping systems. However, it should be noted that the energy consumption in MECs is still high and should be decreased by investigating how the parameters can be optimized to consume less energy. In addition, the comparison between water electrolysis and MECs technologies for hydrogen production showed that WE needs more energy than MECs for the same amount of hydrogen production. In future steps, cost analysis is necessary to be considered to compare the viability of these technologies in comparison with CWTPs. Furthermore, applying SMEC and DMEC as the main wastewater treatment pathway in urban areas has some challenges that should be investigated in future works. For instance, the necessity of pre-treatment and post-treatment systems and their energy consumption to reach high-quality and cost-effective treated water is crucial.

In addition, integrating other potential sustainable energy resources such as wind or sunlight by applying them in a wind turbine or solar panels can provide the required energies to run the bio-electrochemical reactors, making those technologies more reliable and environmentally friendly. Moreover, adding a mathematical model to estimate the exact population and wastewater flow of each district specifying the usage of buildings, including residential and commercial, makes the results more accurate and practical.

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Conflicts of Interest: The authors declare no conflict of interest.

References

1. Alanne, K.; Cao, S. An overview of the concept and technology of ubiquitous energy. *Appl. Energy* **2019**, *238*, 284–302. [CrossRef]
2. Sun, Y.; Shen, C.; Lai, Q.; Liu, W.; Wang, D.-W.; Aguey-Zinsou, K.-F. Tailoring magnesium based materials for hydrogen storage through synthesis: Current state of the art. *Energy Storage Mater.* **2018**, *10*, 168–198. [CrossRef]
3. Pareek, A.; Dom, R.; Gupta, J.; Chandran, J.; Adepu, V.; Borse, P.H. Insights into renewable hydrogen energy: Recent advances and prospects. *Mater. Sci. Energy Technol.* **2020**, *3*, 319–327. [CrossRef]
4. Sdanghi, G.; Maranzana, G.; Celzard, A.; Fierro, V. Review of the current technologies and performances of hydrogen compression for stationary and automotive applications. *Renew. Sustain. Energy Rev.* **2019**, *102*, 150–170. [CrossRef]
5. Dawood, F.; Anda, M.; Shafiullah, G.M. Hydrogen production for energy: An overview. *Int. J. Hydrogen Energy* **2020**, *45*, 3847–3869. [CrossRef]
6. Gielen, D.; Boshell, F.; Saygin, D.; Bazilian, M.D.; Wagner, N.; Gorini, R. The role of renewable energy in the global energy transformation. *Energy Strateg. Rev.* **2019**, *24*, 38–50. [CrossRef]
7. Ursua, A.; Gandia, L.M.; Sanchis, P. Hydrogen production from water electrolysis: Current status and future trends. *Proc. IEEE* **2011**, *100*, 410–426. [CrossRef]
8. Nikolaidis, P.; Poullikkas, A. A comparative overview of hydrogen production processes. *Renew. Sustain. Energy Rev.* **2017**, *67*, 597–611. [CrossRef]
9. Martinez-Burgos, W.J.; de Souza Candeo, E.; Medeiros, A.B.P.; de Carvalho, J.C.; de Andrade Tanobe, V.O.; Soccol, C.R.; Sydney, E.B. Hydrogen: Current advances and patented technologies of its renewable production. *J. Clean. Prod.* **2020**, *286*, 124970. [CrossRef]
10. Saithong, N.; Authayanun, S.; Patcharavorachot, Y.; Arpornwichanop, A. Thermodynamic analysis of the novel chemical looping process for two-grade hydrogen production with CO_2 capture. *Energy Convers. Manag.* **2019**, *180*, 325–337. [CrossRef]
11. Westphal, M.I.; Zhou, L.; Satterthwaite, D.; Martin, S. *Powering Cities in the Global South: How Energy Access for All Benefits the Economy and the Environment*; World Resources Institute: Washington, DC, USA, 2017.
12. Luo, C.; Posen, I.D.; Hoornweg, D.; MacLean, H.L. Modelling future patterns of urbanization, residential energy use and greenhouse gas emissions in Dar es Salaam with the Shared Socio-Economic Pathways. *J. Clean. Prod.* **2020**, *254*, 119998. [CrossRef]
13. Gupta, S.; Srivastava, P.; Patil, S.A.; Yadav, A.K. A comprehensive review on emerging constructed wetland coupled microbial fuel cell technology: Potential applications and challenges. *Bioresour. Technol.* **2021**, *320*, 124376. [CrossRef] [PubMed]
14. Yasri, N.; Roberts, E.P.L.; Gunasekaran, S. The electrochemical perspective of bioelectrocatalytic activities in microbial electrolysis and microbial fuel cells. *Energy Rep.* **2019**, *5*, 1116–1136. [CrossRef]
15. Wilberforce, T.; Sayed, E.T.; Abdelkareem, M.A.; Elsaid, K.; Olabi, A.G. Value added products from wastewater using bioelectrochemical systems: Current trends and perspectives. *J. Water Process Eng.* **2021**, *39*, 101737. [CrossRef]
16. Jafary, T.; Daud, W.R.W.; Ghasemi, M.; Bakar, M.H.A.; Sedighi, M.; Kim, B.H.; Carmona-Martínez, A.A.; Jahim, J.M.; Ismail, M. Clean hydrogen production in a full biological microbial electrolysis cell. *Int. J. Hydrogen Energy* **2019**, *44*, 30524–30531. [CrossRef]
17. Santoro, C.; Arbizzani, C.; Erable, B.; Ieropoulos, I. Microbial fuel cells: From fundamentals to applications. A review. *J. Power Source* **2017**, *356*, 225–244. [CrossRef]
18. Cotterill, S.E.; Dolfing, J.; Jones, C.; Curtis, T.P.; Heidrich, E.S. Low Temperature Domestic Wastewater Treatment in a Microbial Electrolysis Cell with 1 m^2 Anodes: Towards System Scale-Up. *Fuel Cells* **2017**, *17*, 584–592. [CrossRef]
19. Baeza, J.A.; Martínez-Miró, À.; Guerrero, J.; Ruiz, Y.; Guisasola, A. Bioelectrochemical hydrogen production from urban wastewater on a pilot scale. *J. Power Source* **2017**, *356*, 500–509. [CrossRef]

20. Heidrich, E.S.; Dolfing, J.; Scott, K.; Edwards, S.R.; Jones, C.; Curtis, T.P. Production of hydrogen from domestic wastewater in a pilot-scale microbial electrolysis cell. *Appl. Microbiol. Biotechnol.* **2013**, *97*, 6979–6989. [CrossRef]
21. Pinto, R.P.; Srinivasan, B.; Escapa, A.; Tartakovsky, B. Multi-population model of a microbial electrolysis cell. *Environ. Sci. Technol.* **2011**, *45*, 5039–5046. [CrossRef]
22. Mardanpour, M.M.; Yaghmaei, S. Dynamical analysis of microfluidic microbial electrolysis cell via integrated experimental investigation and mathematical modeling. *Electrochim. Acta* **2017**, *227*, 317–329. [CrossRef]
23. Flores-Estrella, R.A.; Rodríguez-Valenzuela, G.; Ramírez-Landeros, J.R.; Alcaraz-González, V.; González-Álvarez, V. A simple microbial electrochemical cell model and dynamic analysis towards control design. *Chem. Eng. Commun.* **2020**, *207*, 493–505. [CrossRef]
24. Alcaraz, V.; Rodriguez, G.; Gomez, J.J.; Dotto, G.L.; Flores, R.A. Hydrogen production automatic control in continuous microbial electrolysis cells reactors used in wastewater treatment. *J. Environ. Manag.* **2021**, *281*, 111869. [CrossRef] [PubMed]
25. Bienvenue sur Montréal.ca. Available online: https://montreal.ca/ (accessed on 15 June 2022).
26. Enright, W.H. The Numerical Analysis of Ordinary Differential Equations: Runge-Kutta and General Linear Methods (JC Butcher). In *Society for Industrial and Applied Mathematics*; John Wiley: Chichester, UK, 1989.
27. Hairer, E.; Wanner, G. Solving Ordinary Differential Equations II. In *Springer Series in Computational Mathematics*; Springer: Berlin/Heidelberg, Germany, 1996; Volume 14. [CrossRef]
28. Maktabifard, M.; Zaborowska, E.; Makinia, J. Achieving energy neutrality in wastewater treatment plants through energy savings and enhancing renewable energy production. *Rev. Environ. Sci. Bio/Technol.* **2018**, *17*, 655–689. [CrossRef]