Numerical simulation of three-dimensional microbial fuel cell

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Abstract. Microbial Fuel Cell (MFC) has various application potential as in generation of bioelectricity, bio-hydrogen production, waste water treatment and it is also used as biosensors. It would not be possible to headway without mentioning that MFCs have quite a many similarities with Chemical Fuel Cells (CFC). It is seen that a lot of research is carried out for CFCs as compared to MFCs. Most of the research works on MFCs include experimental approach while very few computational studies have been carried out for MFCs. So an endeavour is made to create a model which mimics the working by simulating the key physical and biochemical processes occurring. Results imply that variation of current density occurs with change in Reynolds number (Re) and kinetic rate of reaction (k) which lead to the study of effects of variation of flow rates, turbulence and the action of different bacteria in the efficiency of MFCs. The current density achieved computationally is around 512 mA/m² for Re=5 and k=10⁻³ which is in good agreement with the experimental data. Regions of higher current density are found which can be used to improvise the MFCs. Present mathematical model provides a new perspective in understanding the biomass concentration across the MFC and gives better knowledge of the mechanisms taking place. This simple computational framework provides insight into the fluid dynamics involved during continuous feeding, by overcoming the limitations and technical barriers in monitoring and examining through experiments. By implementing the findings from this model optimization of designs can be achieved leading to higher current generation, increase in efficacy and cost effective production techniques which paves the way for future work.

1. Introduction

With the scarcity of the non-renewable sources of energy, it has become a dire need to look for alternative renewable sources and one of such important source is Microbial Fuel Cell (MFC) technology [1]. In MFC, electricity is produced after breaking of organic masses [2] with the help of bacteria. The studies in MFCs received its importance when it was found that domestic water could be treated to practical levels along with simultaneous generation of electricity [3]. The study of application of MFCs started in 1911 [4], however a very little developments were made until recent decades [5, 6]. A great number of research has been done on the Conventional Fuel Cell (CFC) as compared to MFC [7] although a great similarity exists between the two. Proton Exchange Membrane (PEM) [8, 9] is used for separating the anode chamber and cathode chamber and allowing only the positive ion (in this case H⁺ ion) to crossover from anode to cathode side. The process of bacteria generating electrons requires the description of metabolic mechanism. It includes the interaction between bacteria and the reduced/oxidized mediators. This system has quite a similarity to CFC using a Proton Exchange
Membrane which separates the anode and cathode zones. Thus developing a computational model of an MFC cannot be just a simple extension of the already existing fuel cell. Despite of the many similarities in the way the fuel cells operate, there are distinct differences between them that requires a new model to be developed.

MFC has two chambers separated by one membrane, one electrode in each chamber [10, 11, 12]. At anode side, the fuel is supplied that produce H⁺ and electrons, oxidizer is supplied in the cathode side that react with the H⁺ and form water as product. The main difference between CFC and MFC arise in catalyst used and energy source. CFC uses costly materials like platinum as catalyst and Hydrogen or high grade hydrocarbons as energy source, whereas, MFC uses bacteria as its catalyst and various biological materials as the energy source.

One of the biggest advantages that a MFC provide over CFC is the cost put in and its ability to produce electricity along with clean water. However, the most important disadvantage MFC has is the current density which is many orders lower compared to that of CFC [13, 14]. The MFC’s are more sensitive, due to which the chances of breakdown also increase, more maintenance is required. Due to these issues commercialization of MFC is still very difficult. Dynamic simulations are carried out and voltage, power density and fuel concentration are studied [15] and efforts have been made to boost power.

Although many experimental works are carried out for MFC, a clearer picture of the concentration distribution and the fluid dynamics could not be obtained just by monitoring and examining through experiments. On the other hand, a computational framework can help in simulating key physical and biochemical processes by involving detailed numerical study. But a very few numerical studies are available. Thus by building a simplified 3D model an attempt was made to study the effects of feed flow on fluid dynamics and bacteria biological processes involved. This model helped in predicting the biomass concentration in the anode side as well as the current generation during the process. Easy monitoring of the distribution of organics, electrons and protons was achieved and the effects of kinetic rate of reaction and Reynolds number on current generation were studied. Hence this numerical model was effective in overcoming the limitations and technical barriers involved with experiments.

2. Methods of Approach

Knowledge of MFC Technology can be achieved by knowing more about current density, the reaction mechanisms, the numerical methodology and the modelling approach.

2.1. Current Density

The bacteria decompose the nutrients into waste, ions and electron. The ions (H⁺) pass through the membrane and the electrons pass through the circuit and move to the cathode side, resulting in current generation. The number of ions and electrons are assumed to be same and there is no loss. Considering that the electrons can pass through the circuit with very minimum resistance, for every H⁺ ion that has crossed the membrane, the electron that is produced in the anode reaction will also be available at the cathode side moving through the circuit. At steady state, the production of H⁺ at the anode electrode will be same as the consumption of H⁺ ions at the cathode electrode. Assumption is made that anodic oxidation reaction generates 4H⁺ ions per molecule nutrient (Zₐ = 4) and Zc is the number of H⁺ that are consumed on the cathode side. The current (I) produced in a unit of Coulomb/sec I = ZᵥrₐVᵥF where Faradays Constant F is 9.6485x10⁷ (C/kmol) and Vᵥ (m³) refers to the cathode electrode volume. However, a better quantity to describe the performance would be current density (iᵢ), with A as the surface area of the electrodes and x as the thickness of the anode electrode.

\[ i_c = \frac{Z_a e F r_a}{A} = \frac{Z_a Z c F}{A} = Z_a r_a F x \]  

2.2. Reaction Mechanisms in MFC

The overall reaction that is taking place inside this MFC is decomposition of lactate into ions, electrons, waste products, water and possibly carbon dioxide. However, it is not exactly known how and up to what extent the bacteria break the lactate. Products mainly consist of water, hydrogen, carbon monoxide, carbon dioxide, pyruvic acid (C₃H₄O₃), acetate (C₂H₃O₂), formate (HCO₂), and a multitude of other possible species. This computational model will use a simplified reaction with very few species.
As an assumption is made that \( Z_a = 4 \), it implies that an average of 4 moles of \( H^+ \) and electrons for every mole of lactate is consumed at anode electrode. As the exact composition of the exhaust (waste) is not known, it is approximated as a single species rather than a mixture.

\[
C_3H_6O_3 + \text{bacteria} \rightarrow C_3H_2O_3 + 4H^+ + 4e^- 
\]

The net reaction rate for species \( i \) for a non-reversible reaction \( r \) is given by the finite rate model in \( k \) mol/m³-s. As reaction rates varies throughout, integration over the whole reacting area is done.

\[
R_{ltot} = \int_{0}^{L} R_i(x) \, dx 
\]  

(2)

MFC has two volumetric reactions, anodic oxidation reaction producing electron that are consumed in cathodic reduction reaction. Using the Arrhenius expression for stating the forward rate of a reaction and assuming that the MFC is not affected by change of temperature along with zero activation energy, only the constant is obtained which is used as an input variable within a range to see for the variation occurring.

2.3. Numerical Methodology

For getting the desired values, calculation of parameters such as mass fraction, mole fractions, molar concentrations and the density of the individual species and the bulk are carried out. As there are both gaseous and liquid phases in MFC, hence calculation of mixture density is done using volume weighted mixing law. Charge transportation means the transport of \( H^+ \) ions through the membrane and electrons through the circuit. Transportation of \( H^+ \) is considered only through diffusion. However, its molecular weight is very low so it has higher diffusivity than other species, therefore some better transportation properties. Whereas species transport is of nutrient, oxidizer and various other products.

The continuity equation and the Navier Stokes equation for velocity are

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 
\]  

\[
\rho \left[ \frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot (\nabla \vec{V}) \right] = -\nabla p + \mu \nabla^2 (\vec{V}) + f 
\]  

(3)  

(4)

Where \( \vec{V} \) is the flow velocity, \( \rho \) is the density, \( p \) is the pressure, \( \mu \) is the viscosity and \( f \) is the body force. Using the convection-diffusion conservation equation, calculation of the local mass fraction for all the species in the model is done. The conservation equation is given by

\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \vec{V} Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i 
\]  

(5)

Where \( R_i \) denotes the net rate of species \( i \) that is produced by chemical reactions, \( S_i \) denotes the rate of creation due to various sources in the model and \( \vec{J}_i \) the diffusive flux due to concentration gradients.

Considering each species to have a specific diffusion coefficient, the mass diffusion flux for laminar flows becomes

\[
\vec{J}_i = -\rho D_m \frac{\partial Y_i}{\partial x} 
\]  

(6)

The diffusive flux is calculated through user-defined function depending on how the diffusion coefficients \( (D_{l,m}) \) are defined in each section.

2.4. Modelling Approach

Simulations of the MFC are carried out in ANSYS FLUENT [16]. The computational domain of the MFC is of 120.183 mm in length consisting of five zones basically the anode chamber (50 mm), the anode (15 mm), the membrane (0.183 mm), the cathode (5 mm) and the cathode chamber (50 mm) as shown in Figure 1 (a). The cross-section 50 mm × 50 mm is kept constant throughout. The rate of reactions and the boundary conditions are set so as to mimic an actual working MFC which results in oxidation reactions at the anode and reduction reactions at the cathode. However, while doing so, the reactions are assumed to be one directional, occurring at the surfaces and there is no development of biofilm. The entire process is considered isothermal.

3. Results and discussion

By varying different parameters primarily Reynolds number and kinetic rate of reaction, the current density is calculated in each case. The computational results match with the experimental data and follow similar trend as to the available literatures. The experimental data available was without the data of kinetic rate of reaction. Different constant \( C \) (\( C = \frac{C_1}{k} \)) corresponding to the computational data was obtained, which was used to compute kinetic rate of reactions \( k \) (\( k = \frac{I}{C} \)) for the experimental data and
was used to verify the trend as shown in Figure 1 (b). As it can be seen, for different C, the experimental data almost follow the same trend as the numerically computed data obtained from this model. With increase of Reynolds number, there is increase in current density while the kinetic rate of reaction is kept constant as shown in Figure 2 (a).

Similarly, when the Reynolds number is kept constant, with increase in kinetic rate of reaction there is increase in current density as shown in Figure 2 (b). Thus one can conclude that both kinetic rate of reaction and Reynolds number has importance in increasing the current output. However, for Reynolds numbers variation there is no significant change in current density as compared to the case of variation of kinetic rate of reaction. Flow of fluid through the chamber plays an important role, while a very high flow rate will not help in obtaining higher increase in current density. Also it can be seen, the current density values drastically increase with increase in kinetic rate of reaction from $k=10^{-3}$ to $k=10^{-2}$. Thus knowing the optimum value of $k$ can help in increasing the value of current output to a greater extent. Variation of species concentration for $r_1(C_3H_6O_3)$, $r_2(O_2)$, $i(H^+)$, $p_1(C_3H_2O_3)$ and $p_2(H_2O)$ are plotted along $x$-direction for different values of Reynolds number as shown in Figure 3. It can be clearly understood from the plots that not much of a variation lies in concentration of $r_1$ and $r_2$, which are the reactants. While for the products $p_1$, $p_2$ and $i$ variation is evident suggesting decrease in concentration with increase in Reynolds number suggesting that higher rate of flow affects biomass concentration and hence exert influence in lower current generation.

The plotting of isosurfaces as shown in Figure 4 gave an insight about the variation of concentration of various species in the anode, the membrane and the cathode. As shown in Figure 4 (a) the biomass concentration of $C_3H_6O_3$ decreases from the starting of the anode and its concentration becomes very less towards the membrane which verifies the theoretical knowledge. This variation of biomass
concentration across the MFC gives better understanding of the mechanisms taking place. Thus this simple computational framework provides insight into the fluid dynamics involved during continuous feeding, by overcoming the limitations and technical barriers in monitoring and examining through experiments.

Figure 3. Variation of (a) $r_1$ (b) $r_2$ (c) $i$ (d) $p_1$ (e) $p_2$ along $x$ position.

Figure 4. Isosurfaces of (a) $r_1$ (b) $r_2$ (c) $i$ (d) $p_1$ (e) $p_2$

4. Conclusions
Numerical simulations for the three-dimensional MFC are carried out by varying the Reynolds number and the kinetic rate of reaction. The computational data follow a similar trend as to the experimental data. It can be seen that higher the kinetic rate of reaction, higher is the production of current density
when the Reynold number is kept constant. When the kinetic rate of reaction is kept constant, with increase in Reynolds number there is increase in the current density. For Re=5 the current density achieved computationally was around 512 mA/m² at k=10⁻² and 3308 mA/m² at k=10⁻² indicating significant rise just by increase of one order of k. For k=10⁻³ the current density lies within 500-550 mA/m² for Re varying from 0.001 to 10 which suggests not a significant increase was achieved. This mathematical model provided a new perspective in understanding the biomass concentration, bacteria biological processes across the MFC and also knowledge of the fluid dynamics involved during continuous feeding. A good insight of the mechanisms involved are obtained and easy monitoring of the distribution of organics, electrons and protons is achieved. By implementing the findings, optimization of design can be achieved leading to higher current generation and cost effective production.

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References
[1] Logan B E, Hamelers B, Rozendal R, Schröder U, Keller J, Freguia S, Aelterman P, Verstraete W and Rabaey K 2006 Microbial fuel cells: methodology and technology Environ. Sci. & Technol. 40(17) 5181-92.
[2] Lovley D R 2006 Microbial fuel cells: novel microbial physiologies and engineering approaches Current opinion in biotechnology 327-32.
[3] Liu H and Logan B E 2004 Electricity Generation Using an Air-Cathode Single Chamber Microbial Fuel Cell in the Presence and Absence of a Proton Exchange Membrane Environ. Sci Technol. 38 4040-46.
[4] Potter M C 1911 Electrical effects accompanying the decomposition of organic compounds Proc. R. Soc. Lond. Ser. B 84 260-76.
[5] Oh S, Min B and Logan B E 2004 Cathode performance as a factor in electricity generation in microbial fuel cells Environ. Sci. Technol. 38 4900-04.
[6] Xuan J, Leung M K H, Leung D Y C and Ni M 2009 A review of biomass-derived fuel processors for fuel cell systems Renew. and Sustainable Energy Rev. 13 1301-13.
[7] Rittmann B E 2006 Microbial ecology to manage processes in environmental biotechnology Trends in Biotechnol. 24 261-66.
[8] Logan B E, Murano C, Scott K, Gray N D and Head I M 2005 Electricity generation from cysteine in a microbial fuel cell Water Res. 39 942-52.
[9] Rozendal R A, Hamelers H V M and Buisman C J N 2006 Effects of membrane cation transport on pH and microbial fuel cell performance Environ. Sci. Technol. 40 5206-11.
[10] Du F, Xie B, Dong W, Jia B, Dong K and Liu H 2011 Continuous flowing membraneless microbial fuel cells with separated electrode chambers Bioresour. Technol. 102 8914-20.
[11] Picireanu C, Katuri K P, Head I M, Loosdrecht M C M V and Scott K 2008 Mathematical model for microbial fuel cells with anodic biofilms and anaerobic digestion Water Sci. Technol. 57 965-72.
[12] Picireanu C, Loosdrecht M C M V, Curtis T P and Scott K 2010. Model based evaluation of the effect of pH and electrode geometry on microbial fuel cell performance Bioelectrochemistry 78 8-24.
[13] O’hayre R, Cha S W, Prinz F B and Colella W 2016 Fuel cell fundamentals (John Wiley & Sons).
[14] Calder M A 2007 Modeling of a microbial fuel cell (Norwegian University of Science and Technology).
[15] Zeng Y, Choo Y F, Kim B H, Wu P 2009 Modelling and simulation of two-chamber microbial fuel Journal of Power Sources 195 79-89.
[16] Ansys18.0–FLUENT 6.3 User’s Guide.
[17] Logan B E 2008 Microbial fuel cells (John Wiley & Sons).