**Modelling of steady state techno-economic and climate change impact potential saving of Microbial Fuel Cells (MFC)**

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**Background**

Microbial fuel cells (MFC) are a technology for simultaneous removal of chemical oxygen demand (COD) in wastewater in anode chamber and electricity generation from the cell. Electrogenic bacteria harvest electrons and protons utilising organic present in wastewater as substrate in the anode chamber, thereby lowering the COD of the wastewater. Electrons flow through an external circuit from the anode to the cathode chamber generating electricity. In the cathode chamber, electrons and protons combine with oxygen generating net energy output and water. Figure 1 shows MFC schematic.



Figure 1. MFC schematic for electricity generation.

**Steady state overall reaction equation based model**

This section focuses on the mass and energy performance analysis based on the assumption of an overall reaction equation for the MFC. The analysis results are related to the analysis of environmental performance such as global warming potential impact using a life cycle assessment approach and techno-economics. The overall reaction of MFC for electricity generation can be presented as in Equation 1.

Equation 1

The organic substrate in the anode chamber has a chemical formula of , where *x*, *y* and *z* indicate the number of carbon, hydrogen and oxygen atoms, respectively, in 1 mole of substrate.

are the stoichiometric coefficients of substrate, oxygen and water, respectively, in the overall reaction in Equation 1.

From analysed substrate formula, the stoichiometry of the overall reaction in equation 1 can be established, shown in Equations 2-4.

From carbon balance: Equation 2

From hydrogen balance: Equation 3

From oxygen balance: Equation 4

For a given concentration of anode substrate in g/L, volumetric flowrate of wastewater in L/h and fractional conversion of the substrate, , the electricity generation in Watt can be estimated using Equation 5. , and are therefore user inputs that can be varied to conduct sensitivity analysis of their impacts on the outputs in Equations 5 and 7. Atomic mass of carbon, hydrogen and oxygen are 12, ~1 and 16, respectively.

Electricity generation (Watt) under the standard condition =

Equation 5

The standard Gibbs energy of formation of carbon dioxide = -394.36 kJ/mol

The standard Gibbs energy of formation of water = -237.13 kJ/mol

The standard Gibbs free energy of formations of substrate is denoted by (in kJ/mol).

COD and concentration of substrate in g/L are inter-related by Equation 6. Equation 6 is needed to transform between known COD of anode wastewater substrate and concentration of model compound for anode substrate.

Initial COD (g) = Equation 6

The global warming potential to be saved by the MFC is the global warming potential of electricity generation, the service that would be displaced by the MFC. The global warming potential saving by the MFC thus can be estimated at the standard condition (25oC and 1 atm), as shown in Equation 7.

Global warming potential saving by MFC (g CO2 equivalent/h) =

Equation 7

is the global warming potential of electricity generation, the service to be displaced by the MFC, in g CO2 equivalent/kJ electricity generation.

**Techno-economic assessment**

This section discusses the estimation of capital cost of MFC and the discounted cash flow analysis over the life cycle of the MFC1. The capital cost is estimated using Equation 8. In order to arrive at this equation, first the delivered cost of one cell is estimated by the summation of that of each component in the cell, i.e. anode and cathode2. Individual delivered costs are adjusted for the estimated electricity generation rate from a given electricity generation rate. A Lang factor is then applied to estimate the capital cost1-2.

Capital cost = Equation 8

is the delivered cost of each component in a cell, . is the production rate in the same unit as the present production rate (Electricity generation in Equation 5) for the known base size of the component in the cell. Electricity generation estimated using Equation 5 can be transformed into an appropriate unit, e.g. kWh/year, depending on the unit of the . Membrane cost can be a variable and become the main cost contributor. As research effort is on in reducing its cost, economically viable MFC configuration is only considered here.

The net present value () in a given year of the MFC operation is calculated using Equation 93.

Equation 9

is the internal rate of return in fraction. is an (in fraction) applied to the Capital cost (Equation 10). is the operating cost, the summation of the fixed operating cost dependent on the indirect annual capital cost, labour dependent fixed operating cost and the cost of utilities, applied with a multiplier (Equation 11)1. The indirect annual capital cost is dependent on the delivered cost of equipment (Equation 12). The labour dependent fixed operating cost is a function of the production rate (Electricity generation) of the MFC (Equation 13). The cost of utilities includes the cost of anolyte (Equation 14).

Equation 10

Equation 11

Equation 12

Equation 13

are multipliers of the respective cost components to account for a larger set of cost components3.

Equation 14

where,

in Equation 8 is the multiplication between the price of the product (electricity) and its production rate (Equation 15).

Equation 15

For to be in Euro/y, and in Euro/kWh, should be in kWh/y = .

**Case study**

The overall reaction based steady state model of MFC described in Equations 1-7 are exemplified using the anode model substrates. Table 1 shows the relevant input data for some model substrates in anode.

Table 1. Relevant physicochemical and thermochemical data of model substrate compounds in anode. Molar mass and COD are the calculated values.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Anode substrate (s) | *X* | *y* | *z* | (kJ/mol)3 | *molar mass* | *COD, g/mol* | *g COD/g* |
| Acetate | 2 | 3 | 2 | -369.31 | 59 | 56 | 0.95 |
| Glucose | 6 | 12 | 6 | -910 | 180 | 192 | 1.07 |
| Lactate | 3 | 5 | 3 | -516.6 | 89 | 88 | 0.99 |
| Pyruvate | 3 | 3 | 3 | -474.5 | 87 | 72 | 0.83 |
| Sorbitol | 6 | 14 | 6 | -942.7 | 182 | 208 | 1.14 |
| Sucrose | 12 | 22 | 11 | -1551.8 | 342 | 384 | 1.12 |

Equations 2-7 are exemplified for the anode model substrates in Table 1, as shown in Table 2. Table 2 shows the calculated outputs of Equations 2-5 and 7.

For the following values, concentration of anode substrate = 1 g/L, volumetric flowrate of wastewater = 1 L/h and fractional conversion of the substrate = 0.7, Table 2 shows the calculated outputs of Equations 2-5 and 7, for all the chosen anode substrates in Table 1. is calculated using equal proportions of all energy source or technology options and the factors applied for the estimation of the GWP of the UK grid electricity mix5 (Table 3)

Table 2. Outputs of Equations 2-5 and 7, for all the chosen anode substrates in Table 1 and concentration of anode substrate = 1 g/L, volumetric flowrate of wastewater = 1 L/h and fractional conversion of the substrate = 0.7.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Anode substrate | x' | n' | n | Electricity generation (Watt) | GWP saving in g CO2 equivalent/h |
| Acetate | 0.50 | 0.75 | 0.88 | 2.55 | 0.82 |
| Glucose | 0.17 | 1.00 | 1.00 | 3.11 | 0.99 |
| Lactate | 0.33 | 0.83 | 0.92 | 2.75 | 0.88 |
| Pyruvate | 0.33 | 0.50 | 0.75 | 2.38 | 0.76 |
| Sorbitol | 0.17 | 1.17 | 1.08 | 3.29 | 1.05 |
| Sucrose | 0.08 | 0.92 | 1.00 | 3.29 | 1.05 |

Table 3. of energy source or technology options5.

|  |  |
| --- | --- |
|  | kg CO2 equivalent/MJ |
| CCGT | 0.1386 |
| Nuclear | 0.0081 |
| Biomass | 0.0125 |
| Coal | 0.2467 |
| Wind | 0.0072 |
| Solar | 0.0236 |
| Oil | 0.2036 |
| OCGT | 0.1386 |
| Hydroelectric | 0.0072 |
| Pumped hydro | 0.1153 |
| Other | 0.0758 |

The techno-economic analysis model shown in Equations 8-15 is applied to all the combinations, anode substrates of choice in Table 1. The user input variables for the techno-economic analysis model are shown in Table 4.

Table 4. User input parameters for techno-economic analysis2.

|  |  |  |  |
| --- | --- | --- | --- |
| **Delivered cost** | **Default** | **Unit** | **Range** |
| Anode | 15 | Euro/m2 | 5-20 |
| Cathode | 15 | Euro/m2 | 5-20 |
|  |  |  |  |
| Lang factor | 1.5 |  | 1-2 |
|  |  |  |  |
| **Variables for NPV calculations** |  |  |  |
|  | 0.13 |  | 0.05-0.15 |
| IRR | 0.12 |  | 0.05-0.15 |
|  |  |  |  |
| **Price of utility** |  |  |  |
| Anolyte | 0.0012 | Euro/m3 | 0.001-0.002 |
| Catholyte | 0.5 | Euro/m3 | 0.1-1 |
|  |  |  |  |
| **Electricity price** | 0.15 | Euro/kWh | 0.05-0.2 |

= 0.0016 m2 for anode and cathode for a = 0.017 Watt. Thus, the power density of MFC is 10.8 Watt/m2. These values are applied in Equation 8 to estimate the capital costs for the various anode substrates of choice in Table 1, as shown in Table 5.

Table 5. Estimated capital cost using Equation 8 for the various anode substrates of choice in Table 1, and concentration of anode substrate = 1 g/L, volumetric flowrate of wastewater = 1 L/h and fractional conversion of the substrate = 0.7.

|  |  |
| --- | --- |
| Anode substrate | Capital cost (Euro) |
| Acetate | 10.60 |
| Glucose | 12.90 |
| Lactate | 11.42 |
| Pyruvate | 9.87 |
| Sorbitol | 13.67 |
| Sucrose | 13.66 |

For Equations 11 and 13, the dimensionless multiplier values are: 1.3, 0.19 and 0.09 (when the substrate flowrate is in g/h), respectively1. See Appendix A for the derivation of the dimensionless multiplier values. The consumption rate of anolyte and catholyte can be estimated proportionally for the present electricity generation based on the following data: a cell volume of 0.29 L gives a = 0.017 Watt (Equation 14)2. Equations 8-15 further use the input cost or price data in Table 4. The discounted cash flow (Equation 9) with respect to year over the MFC life is estimated for acetate as the model substrate of anode, as shown in Figure 2.

Figure 2. Discounted cash flow analysis of MFC for acetate as the model substrate of anode.

The total cost () (in Euro/year) divided by the power generation (in kWh/year) (Table 2) gives the minimum selling price of electricity, estimated at 0.07 Euro/kWh, lower than the price of electricity (Table 4), thus, making the MFC profitable.

**References**

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2. Shemfe, M., Gadkari, S., Yu, E., Rasul, S., Scott, K., Head, I.M., Gu, S. and Sadhukhan, J., 2018. Life cycle, techno-economic and dynamic simulation assessment of bioelectrochemical systems: A case of formic acid synthesis. *Bioresource technology*, *255*, pp.39-49.
3. Sadhukhan, J., Lloyd, J.R., Scott, K., Premier, G.C., Eileen, H.Y., Curtis, T. and Head, I.M., 2016. A critical review of integration analysis of microbial electrosynthesis (MES) systems with waste biorefineries for the production of biofuel and chemical from reuse of CO2. *Renewable and Sustainable Energy Reviews*, *56*, pp.116-132.
4. Extracted from SimaPro 9 Ecoinvent 3.6.
5. <https://gridwatch.co.uk/co2-Emissions>
6. Sadhukhan, J., Martinez-Hernandez, E., Amezcua-Allieri, M.A. and Aburto, J., 2019. Economic and environmental impact evaluation of various biomass feedstock for bioethanol production and correlations to lignocellulosic composition. *Bioresource Technology Reports*, *7*, p.100230.

**Appendix A (Please Refer to Chapter 2 of Reference 1. Sadhukhan, J. Ng, K.S. and Martinez-Hernandez, E., 2014. *Biorefineries and Chemical Processes: Design, Integration and Sustainability Analysis*. Wiley, Chichester, UK. for economic analysis calculations.)**

The operating costs can be classified into two main categories: fixed and variable operating costs. Fixed operating costs are independent of the production rate and quantity, in contrast to variable operating costs. This includes the costs of maintenance, labour, taxation, insurance, royalties etc. Fixed operating costs are estimated using factors, normally based on indirect capital cost and labour cost. Variable operating costs consist of the costs of raw materials, utilities etc. The sum of fixed and variable operating costs is the Direct Production Costs (DPC) of a plant. Other costs such as the costs of research and development, sales expenses and general overheads are added as % of DPC to obtain the total operating cost. The total operating cost is usually 1.2 or 1.3 times the DPC. Thus, the value of in Equation 11 is 1.3. The accounting of these cost items is shown in Equation A1.

Equation A1

The indirect capital cost is 1.26 times the delivered cost of equipment for solid-fluid processing system. The indirect capital cost includes the following cost items: engineering and supervision, construction expenses, legal expenses, contractor’s fee and contingency. Furthermore, the fixed operating cost dependent on the indirect capital cost is 0.15 times the indirect capital cost. The fixed operating cost dependent on the indirect capital cost includes the following cost items: maintenance, capital charges, insurance, local taxes and royalties. Thus, the value of in Equation 11 is .

The fixed operating cost dependent on the personnel cost is 1.9 times the personnel cost. The fixed operating cost dependent on the personnel cost includes the following cost items: labour, laboratory, supervision and plant overheads. The personnel cost is $52033 per t/h substrate flowrate6. 1 EURO is assumed to be 0.9 times $1. Thus, the value of in Equation 13 is .